

## TESTING CONDITIONAL INDEPENDENCE USING MAXIMAL NONLINEAR CONDITIONAL CORRELATION<sup>1,2,3</sup>

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In this paper, the maximal nonlinear conditional correlation of two random vectors  $X$  and  $Y$  given another random vector  $Z$ , denoted by  $\rho_1(X, Y|Z)$ , is defined as a measure of conditional association, which satisfies certain desirable properties. When  $Z$  is continuous, a test for testing the conditional independence of  $X$  and  $Y$  given  $Z$  is constructed based on the estimator of a weighted average of the form  $\sum_{k=1}^n f_Z(z_k) \rho_1^2(X, Y|Z = z_k)$ , where  $f_Z$  is the probability density function of  $Z$  and the  $z_k$ 's are some points in the range of  $Z$ . Under some conditions, it is shown that the test statistic is asymptotically normal under conditional independence, and the test is consistent.

**1. Introduction.** In this paper, the problem of interest is testing the conditional independence between two random vectors  $X$  and  $Y$  given a third random vector  $Z$ . The study of the problem of testing conditional independence has a long history. However, there are relatively few results on nonparametric tests when the vectors  $X$ ,  $Y$  and  $Z$  are continuous. Some examples of such tests can be found in Su and White [12, 13], where they also proposed conditional independence tests based on a weighted Hellinger distance between the conditional densities or the difference between the conditional characteristic functions.

As mentioned in Daudin [2],  $X$  and  $Y$  are conditionally independent given  $Z$  means that for every  $f(X, Z)$  and  $g(Y, Z)$  such that  $Ef^2(X, Z)$

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and  $Eg^2(Y, Z)$  are finite

$$E(f(X, Z)g(Y, Z)|Z) = E(f(X, Z)|Z)E(g(Y, Z)|Z).$$

Thus, the problem of testing conditional independence, as the problem of testing unconditional independence, is invariant when one-to-one transforms are applied to the marginals  $X$  and  $Y$ , respectively. Various authors have taken this invariant property into consideration when constructing conditional or unconditional independence tests. For example, Su and White [13] used Hellinger distance in their test statistic for testing conditional independence, so that the test statistic is invariant. Dauxois and Nkiet [3] used measures of association to construct independence tests, and the measures are invariant under the above transforms. In this paper, to take invariance into account, the proposed test is based on the maximal nonlinear conditional correlation, which can be viewed as a measure of conditional association and satisfies the above invariance property.

To choose a reasonable measure of conditional association between  $X$  and  $Y$ , the following properties are considered.

- (P1) The measure can be defined for all types of random vectors, including both discrete and continuous ones.
- (P2) The measure is symmetric, that is, it remains the same when  $(X, Y)$  is replaced by  $(Y, X)$ .
- (P3) The measure is invariant when one-to-one transforms are applied to  $X$  and  $Y$ , respectively.
- (P4) The measure is between 0 and 1.
- (P5) The measure is 0 if and only if conditional independence holds.

The above properties are adapted from some of the conditions for a good measure of association proposed by Rényi [9]. In [9], the conditional independence in (P5) is replaced by the unconditional independence. Note that the symmetric property (P2) is not always required. For instance, Hsing et al. [6] proposed to use the coefficient of intrinsic dependence as a measure of dependence, which does not satisfy (P2). Here, (P2) is considered.

Many measures of conditional association satisfying (P1)–(P5) can be constructed. Dauxois and Nkiet [4] showed that a class of measures of association between two Hilbertian subspaces can be obtained by properly combining the canonical coefficients of the canonical analysis (CA) between the spaces. In particular, take the two subspaces to be  $\tilde{H}_1 = \{f(X, Z) - E(f(X, Z)|Z) : Ef^2(X, Z) < \infty\}$  and  $\tilde{H}_2 = \{g(Y, Z) - E(g(Y, Z)|Z) : Eg^2(Y, Z) < \infty\}$ , then a class of measures of conditional association between  $X$  and  $Y$  given  $Z$  satisfying properties (P1)–(P5) can be obtained using the canonical coefficients. Denote the canonical coefficients (arranged in descending order) by  $\tilde{\rho}_i(X, Y|Z) : i = 1, 2, \dots$ . When  $X$  and  $Y$  are not

functions of  $Z$ , the largest canonical coefficient  $\tilde{\rho}_1(X, Y|Z)$  is the maximal partial correlation defined by Romanovič [10], which is

$$\sup_{f,g} \text{corr}(f(X, Z) - E(f(X, Z)|Z), g(Y, Z) - E(g(Y, Z)|Z)).$$

Another approach to construct measures of conditional association is to modify the CA between the spaces  $H_1 = \{f(X) - Ef(X) : Ef^2(X) < \infty\}$  and  $H_2 = \{g(Y) - Eg(Y) : Eg^2(Y) < \infty\}$  to obtain a conditional version of it. That is, to find pairs of functions  $(f_i, g_i) : i = 0, 1, \dots$ , such that for each  $i$ ,  $(f_i, g_i)$  maximizes  $E(f(X, Z)g(Y, Z)|Z)$  subject to

$$(1.1) \quad E(f^2(X, Z)|Z)I_{(0,\infty)}(E(f^2(X, Z)|Z)) = I_{(0,\infty)}(E(f^2(X, Z)|Z)),$$

$$(1.2) \quad E(g^2(Y, Z)|Z)I_{(0,\infty)}(E(g^2(Y, Z)|Z)) = I_{(0,\infty)}(E(g^2(Y, Z)|Z))$$

and

$$E(f(X, Z)f_j(X, Z)|Z) = 0 = E(g(Y, Z)g_j(Y, Z)|Z) \quad \text{for } 0 \leq j < i.$$

Here,  $I_A$  denotes the indicator function on a set  $A$ , that is,  $I_A(x) = 1$  if  $x \in A$  and  $I_A(x) = 0$ , otherwise. If the above  $(f_i, g_i)$ 's exist, then one can define  $\rho_i(X, Y|Z) = E(f_i(X, Z)g_i(Y, Z)|Z)$  for each  $i$  and the  $\rho_i(X, Y|Z)$ 's can serve as a conditional version of canonical coefficients. A measure of conditional association satisfying (P1)–(P5) can be obtained by taking a proper combination of the  $\rho_i(X, Y|Z)$ 's, following the approach in [4]. Examples of such combinations include  $\rho_1(X, Y|Z)$  and  $1 - \exp(-\sum_i \rho_i^2(X, Y|Z))$ . The measure of conditional association used in this paper is  $\rho_1(X, Y|Z)$ , which will be called the maximal nonlinear conditional correlation of two random vectors  $X$  and  $Y$  given  $Z$  from now on.

In the above definition of  $\rho_i(X, Y|Z)$ 's, it is assumed that the  $(f_i, g_i)$ 's exist. However, it is not clear what conditions can guarantee the existence of the  $(f_i, g_i)$ 's. To avoid the problem of finding such conditions, a more general definition for  $\rho_1(X, Y|Z)$  is given in Section 2. To construct a test based on  $\rho_1(X, Y|Z)$ , it is assumed that  $Z$  has a Lebesgue probability density function  $f_Z$ . An estimator of  $\sum_k f_Z(z_k)\rho_1^2(X, Y|Z = z_k)$  is then used as the test statistic, where the  $z_k$ 's are some points in the range of  $Z$ . To study the asymptotic behavior of the test statistic under the hypothesis that  $X$  and  $Y$  are conditionally independent given  $Z$ , we follow the approach in [3] for finding the asymptotic distribution of a statistic for testing the independence between  $X$  and  $Y$ , which is based on estimators of the canonical coefficients from the CA of  $H_1$  and  $H_2$ . To make the approach work for the conditional case, some strong approximation results for kernel estimators of certain conditional expectations are also established.

This paper is organized as follows. The new definition of  $\rho_1(X, Y|Z)$  is given in Section 2. Section 3 deals with the estimation of  $\rho_1(X, Y|Z = z)$  and test construction. An example is in Section 4 and proofs are given in Section 7.

**2. Maximal nonlinear conditional correlation.** In this section, a more general definition of the maximal nonlinear conditional correlation  $\rho_1(X, Y|Z)$  will be given. Note that in the definition of  $\rho_i(X, Y|Z)$ 's in Section 1, one can take  $f_0(X, Z) = 1 = g_0(Y, Z)$ , which gives that  $\rho_0(X, Y|Z) = 1$ , and then  $\rho_1(X, Y|Z)$  can be defined as  $E(f_1(X, Z)g_1(Y, Z)|Z)$  if there exists  $(f_1, g_1) \in S_0$  such that

$$E(f(X, Z)g(Y, Z)|Z) \leq E(f_1(X, Z)g_1(Y, Z)|Z) \quad \text{for every } (f, g) \in S_0,$$

where  $S_0$  is the collection of pairs of functions  $(f, g)$ 's that satisfy (1.1), (1.2) and  $E(f(X, Z)|Z) = 0 = E(g(Y, Z)|Z)$ . Without assuming the existence of  $(f_1, g_1)$ , it is reasonable to define  $\rho_1(X, Y|Z)$  as

$$(2.1) \quad \sup_{(f, g) \in S_0} E(f(X, Z)g(Y, Z)|Z),$$

if the supremum can be defined.

The above approach can be considered as a “pointwise” approach. Indeed, when  $Z$  takes values in a countable set  $\mathcal{Z}$ , for each  $z \in \mathcal{Z}$ , one may define  $\rho_1(X, Y|Z = z)$  as

$$(2.2) \quad \sup_{(f, g) \in S_0} E(f(X, z)g(Y, z)|Z = z),$$

then the  $\rho_1(X, Y|Z)$  defined using (2.2) is a measurable function and can serve as the supremum in (2.1). However, if  $\mathcal{Z}$  is uncountable, then it is not clear whether the  $\rho_1(X, Y|Z)$  defined using (2.2) is measurable. Therefore, we use the following fact to define the supremum in (2.1) so that it is well defined and is a measurable function.

FACT 1. *There exists a sequence  $\{(\alpha_n, \beta_n)\}$  in  $S_0$  such that:*

- (i) *The sequence  $\{E(\alpha_n(X, Z)\beta_n(Y, Z)|Z)\}$  is nondecreasing, and*
- (ii) *for every  $(f, g) \in S_0$ ,*

$$E(f(X, Z)g(Y, Z)|Z) \leq \lim_{n \rightarrow \infty} E(\alpha_n(X, Z)\beta_n(Y, Z)|Z).$$

Furthermore, if (i) and (ii) hold for  $\{(\alpha_n, \beta_n)\} = \{(\alpha_{n,1}, \beta_{n,1})\}$  or  $\{(\alpha_{n,2}, \beta_{n,2})\}$ , where  $\{(\alpha_{n,1}, \beta_{n,1})\}$  and  $\{(\alpha_{n,2}, \beta_{n,2})\}$  are sequences in  $S_0$ , then

$$(2.3) \quad \lim_{n \rightarrow \infty} E(\alpha_{n,1}(X, Z)\beta_{n,1}(Y, Z)|Z) = \lim_{n \rightarrow \infty} E(\alpha_{n,2}(X, Z)\beta_{n,2}(Y, Z)|Z).$$

For the sake of brevity, from now on, some functions of  $(X, Z)$  or  $(Y, Z)$  may be expressed without the arguments  $(X, Z)$  or  $(Y, Z)$ . For distinguishing purpose, functions of  $(X, Z)$  may have names starting with only  $\alpha$  or  $f$ , and functions of  $(Y, Z)$  may have names starting with only  $\beta$  or  $g$ .

PROOF FOR FACT 1. We will first establish (2.3) if (i) and (ii) hold for  $\{(\alpha_n, \beta_n)\} = \{(\alpha_{n,1}, \beta_{n,1})\}$  or  $\{(\alpha_{n,2}, \beta_{n,2})\}$ . Note that for each  $n$ , from (ii), we have that

$$E(\alpha_{n,2}\beta_{n,2}|Z) \leq \lim_{n \rightarrow \infty} E(\alpha_{n,1}\beta_{n,1}|Z)$$

and

$$E(\alpha_{n,1}\beta_{n,1}|Z) \leq \lim_{n \rightarrow \infty} E(\alpha_{n,2}\beta_{n,2}|Z).$$

Take the limits in these two inequalities as  $n \rightarrow \infty$ , and we have (2.3).

It remains to find a sequence  $\{(\alpha_n, \beta_n)\}$  in  $S_0$  that satisfies (i) and (ii). Let  $\{(\alpha_{n,0}, \beta_{n,0})\}$  be a sequence in  $S_0$  so that the sequence  $\{E(\alpha_{n,0}\beta_{n,0})\}$  is non-decreasing and converges to  $\sup_{(f,g) \in S_0} E(fg)$ . We will construct  $\{(\alpha_n, \beta_n)\}$  using  $\{(\alpha_{n,0}, \beta_{n,0})\}$  as follows. For  $n = 1$ , define  $(\alpha_1, \beta_1) = (\alpha_{1,0}, \beta_{1,0})$ . For  $n \geq 2$ , define

$$\begin{aligned} & (\alpha_n(X, Z), \beta_n(Y, Z)) \\ &= \begin{cases} (\alpha_{n,0}(X, Z), \beta_{n,0}(Y, Z)), & \text{if } E(\alpha_{n,0}\beta_{n,0}|Z) > E(\alpha_{n-1}\beta_{n-1}|Z); \\ (\alpha_{n-1}(X, Z), \beta_{n-1}(Y, Z)), & \text{otherwise.} \end{cases} \end{aligned}$$

Then  $\{(\alpha_n, \beta_n)\}$  is a sequence in  $S_0$  that satisfies (i), and the sequence  $\{E\alpha_n\beta_n\}$  converges to  $\sup_{(f,g) \in S_0} E(fg)$  since  $E(\alpha_n\beta_n|Z) \geq E(\alpha_{n,0}\beta_{n,0}|Z)$ . To see that  $\{(\alpha_n, \beta_n)\}$  also satisfies (ii), for  $(\alpha, \beta)$  in  $S_0$ , define

$$(\alpha_n^*, \beta_n^*) = \begin{cases} (\alpha, \beta), & \text{if } E(\alpha\beta|Z) > \lim_{n \rightarrow \infty} E(\alpha_n\beta_n|Z); \\ (\alpha_n, \beta_n), & \text{otherwise.} \end{cases}$$

Then  $\{(\alpha_n^*, \beta_n^*)\}$  is a sequence in  $S_0$  such that

$$(2.4) \quad \lim_{n \rightarrow \infty} E(\alpha_n^*\beta_n^*|Z) = \max\left\{E(\alpha\beta|Z), \lim_{n \rightarrow \infty} E(\alpha_n\beta_n|Z)\right\}.$$

From the monotone convergence theorem, we have

$$(2.5) \quad E \lim_{n \rightarrow \infty} E(\alpha_n^*\beta_n^*|Z) = \lim_{n \rightarrow \infty} E(\alpha_n^*\beta_n^*)$$

and

$$(2.6) \quad E \lim_{n \rightarrow \infty} E(\alpha_n\beta_n|Z) = \lim_{n \rightarrow \infty} E(\alpha_n\beta_n),$$

so (2.4) implies that

$$\sup_{(f,g) \in S_0} E(fg) \geq \lim_{n \rightarrow \infty} E(\alpha_n^*\beta_n^*) \geq \lim_{n \rightarrow \infty} E(\alpha_n\beta_n) = \sup_{(f,g) \in S_0} E(fg),$$

which gives

$$(2.7) \quad \lim_{n \rightarrow \infty} E(\alpha_n^*\beta_n^*) = \lim_{n \rightarrow \infty} E(\alpha_n\beta_n).$$

If  $E(\alpha\beta|Z) > \lim_{n \rightarrow \infty} E(\alpha_n\beta_n|Z)$  with positive probability, then (2.4), (2.5) and (2.6) together implies that  $\lim_{n \rightarrow \infty} E(\alpha_n^*\beta_n^*) > \lim_{n \rightarrow \infty} E(\alpha_n\beta_n)$ , which contradicts (2.7). Thus, (ii) holds. The proof of Fact 1 is complete.  $\square$

With Fact 1, the maximal nonlinear conditional correlation  $\rho_1(X, Y|Z)$  can be redefined as follows.

**DEFINITION 1.**  $\rho_1(X, Y|Z) = \sup_{(f,g) \in S_0} E(f(X, Z)g(Y, Z)|Z)$ , which is defined as  $\lim_{n \rightarrow \infty} E(\alpha_n(X, Z)\beta_n(Y, Z)|Z)$ , where  $\{(\alpha_n, \beta_n)\}$  is a sequence in  $S_0$  that satisfies (i) and (ii) in Fact 1.

Below are some remarks for the  $\rho_1(X, Y|Z)$ .

1. If there exists  $(f_1, g_1)$  in  $S_0$  such that  $E(f_1g_1|Z) \geq E(fg|Z)$  for all  $(f, g) \in S_0$ , then  $\rho_1(X, Y|Z) = E(f_1g_1|Z)$  using Definition 1. To see this, let  $\{(\alpha_n, \beta_n)\}$  be a sequence in  $S_0$  that satisfies (i) and (ii) in Fact 1. Then  $\rho_1(X, Y|Z) = \lim_{n \rightarrow \infty} E(\alpha_n\beta_n|Z)$ , so  $E(f_1g_1|Z) \leq \rho_1(X, Y|Z)$  by (ii). Also,  $E(f_1g_1|Z) \geq E(\alpha_n\beta_n|Z)$  for every  $n$ , so  $E(f_1g_1|Z) \geq \rho_1(X, Y|Z)$ . Therefore,  $\rho_1(X, Y|Z) = E(f_1g_1|Z)$  and Definition 1 can be viewed as a generalized version of the definition of  $\rho_1(X, Y|Z)$  given in Section 1.
2.  $\rho_1(X, Y|Z)$  satisfies properties (P1)–(P5).
3. When  $X$  is a function of  $Y$  and  $Z$  or  $Y$  is a function of  $X$  and  $Z$ , it is not necessary that  $\rho_1(X, Y|Z) = 1$ . For instance, suppose that  $X$  and  $Z$  are independent standard normal random variables and  $Y = XI_{(0, \infty)}(Z)$ , then  $\rho_1(X, Y|Z) = I_{(0, \infty)}(Z)$ .
4. Let  $\rho_1(X, Y)$  be the largest canonical coefficient from the CA between  $H_1 = \{f(X) - Ef(X) : Ef^2(X) < \infty\}$  and  $H_2 = \{g(Y) - Eg(Y) : Eg^2(Y) < \infty\}$ . Then  $\rho_1(X, Y|Z) = \rho_1(X, Y)$  if  $(X, Y)$  and  $Z$  are independent.
5. Let  $\rho_1(X, Y)$  be as defined in item 4. It is stated in [3] that when the joint distribution of  $X$  and  $Y$  is bivariate normal

$$N\left(\begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 1 & \rho \\ \rho & 1 \end{pmatrix}\right),$$

$\rho_1(X, Y) = |\rho|$ . This result implies that, when the joint distribution for  $X$ ,  $Y$  and  $Z$  is multivariate normal and  $X$  and  $Y$  are both univariate,

$$\begin{aligned} \rho_1(X, Y|Z) &= \left| \frac{E((X - E(X|Z))(Y - E(Y|Z))|Z)}{(E(X - E(X|Z))^2|Z)^{1/2}(E(Y - E(Y|Z))^2|Z)^{1/2}} \right| \\ &= \left| \frac{E(X - E(X|Z))(Y - E(Y|Z))}{(E(X - E(X|Z))^2)^{1/2}(E(Y - E(Y|Z))^2)^{1/2}} \right|, \end{aligned}$$

which also equals the absolute value of the usual partial correlation coefficient.

**3. A test of conditional independence.** Testing conditional independence is equivalent to testing  $H_0: \rho_1(X, Y|Z) = 0$ , which involves testing  $H_{0,z}: \rho_1(X, Y|Z = z) = 0$  for different  $z$ 's in the range of  $Z$ . Let  $\mathcal{Z}$  be the range of  $Z$ . In this section, an estimator  $\hat{\rho}(z)$  is proposed for estimating  $\rho_1(X, Y|Z = z)$  for each  $z \in \mathcal{Z}$ , and for distinct points  $z_1, \dots, z_{n_Z}$  in  $\mathcal{Z}$ , the asymptotic joint distribution of  $\hat{\rho}(z_1), \dots, \hat{\rho}(z_{n_Z})$  under  $H_0$  is derived to construct a test for testing  $H_0$ .

3.1. *Estimation of  $\rho_1(X, Y|Z = z)$ .* To estimate

$$\rho_1(X, Y|Z) = \sup_{(f,g) \in S_0} E(fg|Z)$$

for  $(f, g) \in S_0$ ,  $f$  and  $g$  are approximated using basis functions. Suppose that there exist  $\Lambda_1$ ,  $\Lambda_2$  and  $\Lambda_3$ : subsets of the set of all positive integers and three sets of functions  $\{\phi_{p,i}: 1 \leq i \leq p, p \in \Lambda_1\}$ ,  $\{\psi_{q,j}: 1 \leq j \leq q, q \in \Lambda_2\}$  and  $\{\theta_{r,k}: 1 \leq k \leq r, k \in \Lambda_3\}$  such that for  $\alpha(X, Z)$  and  $\beta(Y, Z)$  with finite second moments,

$$(3.1) \quad \lim_{p,r \rightarrow \infty} \inf_{a(i,k)} E \left( \alpha(X, Z) - \sum_{1 \leq i \leq p, 1 \leq k \leq r} a(i, k) \phi_{p,i}(X) \theta_{r,k}(Z) \right)^2 = 0$$

and

$$(3.2) \quad \lim_{q,r \rightarrow \infty} \inf_{b(j,k)} E \left( \beta(Y, Z) - \sum_{1 \leq j \leq q, 1 \leq k \leq r} b(j, k) \psi_{q,j}(Y) \theta_{r,k}(Z) \right)^2 = 0.$$

Also, suppose that for each  $(p, q)$ , there exist coefficients  $a_{p,0,i}$ 's and  $b_{q,0,j}$ 's such that

$$(3.3) \quad \sum_{1 \leq i \leq p} a_{p,0,i} \phi_{p,i}(x) = 1 = \sum_{1 \leq j \leq q} b_{q,0,j} \psi_{q,j}(y)$$

for every  $x$  in the range of  $X$  and every  $y$  in the range of  $Y$ .

Let  $S_1$  be the collection of all  $(f, g)$ 's with finite second moments and let  $S_{1,p,q}$  be the collection of all  $(f, g)$ 's in  $S_1$  such that  $f(X, Z) = \sum_{i=1}^p a_{p,i}(Z) \phi_{p,i}(X)$  for some  $a_{p,i}(Z)$ 's, and  $g(Y, Z) = \sum_{j=1}^q b_{q,j}(Z) \psi_{q,j}(Y)$  for some  $b_{q,j}(Z)$ 's. Then (3.1) and (3.2) together imply that  $S_1$  can be approximated by  $S_{1,p,q}$  for large  $p$  and  $q$ . Since  $S_0 \subset S_1$ ,  $S_0$  can be approximated by  $S_{1,p,q}$  as well. With the additional condition (3.3),  $S_0$  can be easily approximated using the subspace  $S_{0,p,q} = S_0 \cap S_{1,p,q}$ . Note that (3.1), (3.2) and (3.3) hold for certain basis functions, for example, the tensor product splines in [11].

Assuming (3.1), (3.2) and (3.3), it is reasonable to define

$$\sup_{(f,g) \in S_{0,p,q}} E(fg|Z)$$

and use it to approximate  $\rho_1(X, Y|Z)$ . To define  $\sup_{(f,g) \in S_{0,p,q}} E(fg|Z)$ , one may follow the same approach for defining  $\sup_{(f,g) \in S_0} E(fg|Z)$ , or simply note that there exists  $(f_1, g_1) \in S_{0,p,q}$  such that

$$(3.4) \quad E(f_1 g_1 | Z) \geq E(fg | Z) \quad \text{for all } (f, g) \in S_{0,p,q}$$

and define  $\sup_{(f,g) \in S_{0,p,q}} E(fg|Z) = E(f_1 g_1 | Z)$ . The pair  $(f_1, g_1)$  can be obtained as follows. Let

$$\Sigma_{\phi,p}(Z) = (E(\phi_{p,i}(X)\phi_{p,j}(X)|Z) - E(\phi_{p,i}(X)|Z)E(\phi_{p,j}(X)|Z))_{p \times p},$$

$$\Sigma_{\psi,q}(Z) = (E(\psi_{q,i}(Y)\psi_{q,j}(Y)|Z) - E(\psi_{q,i}(Y)|Z)E(\psi_{q,j}(Y)|Z))_{q \times q}$$

and

$$\Sigma_{\phi,\psi,p,q}(Z) = (E(\phi_{p,i}(X)\psi_{q,j}(Y)|Z) - E(\phi_{p,i}(X)|Z)E(\psi_{q,j}(Y)|Z))_{p \times q}.$$

Consider the following two cases:

- (i)  $\Sigma_{\phi,p}(Z)$  and  $\Sigma_{\psi,q}(Z)$  are not zero matrices, and
- (ii) at least one of  $\Sigma_{\phi,p}(Z)$  and  $\Sigma_{\psi,q}(Z)$  is a zero matrix.

In case (i), let  $a_1 = (a_{1,1}(Z), \dots, a_{1,p}(Z))^T$  and  $b_1 = (b_{1,1}(Z), \dots, b_{1,q}(Z))^T$  be such that  $(a_1, b_1)$  is the pair of  $(a, b)$  that maximizes

$$a^T \Sigma_{\phi,\psi,p,q}(Z) b$$

subject to

$$a^T \Sigma_{\phi,p}(Z) a = 1 = b^T \Sigma_{\psi,q}(Z) b,$$

and then take

$$f_1(X, Z) = \sum_{i=1}^p a_{1,i}(Z) (\phi_{p,i}(X) - E(\phi_{p,i}(X)|Z))$$

and

$$g_1(Y, Z) = \sum_{j=1}^q b_{1,j}(Z) (\psi_{q,j}(Y) - E(\psi_{q,j}(Y)|Z)).$$

In case (ii), take  $f_1(X, Z) = 0 = g_1(Y, Z)$ . Then  $(f_1, g_1) \in S_{0,p,q}$  and (3.4) holds. Denote  $\sup_{(f,g) \in S_{0,p,q}} E(fg|Z)$  by  $\rho_{p,q}(Z)$ .

The following fact states that  $\rho_1(X, Y|Z)$  can be reasonably approximated by  $\rho_{p,q}(Z)$  if  $p$  and  $q$  are large.

**FACT 2.** *Suppose that (3.1), (3.2) and (3.3) hold and  $\{p_n\}$  and  $\{q_n\}$  are sequences of positive integers that tend to  $\infty$  as  $n \rightarrow \infty$ . Then*

$$\lim_{n \rightarrow \infty} E(|\rho_1(X, Y|Z) - \rho_{p_n, q_n}(Z)|) = 0.$$



PROOF. Since  $\rho_1(X, Y|Z) \geq \rho_{p_n, q_n}(Z)$  for every  $n$ , Fact 2 holds if for every  $\varepsilon > 0$ , there exists  $N_0$  such that for  $n \geq N_0$ ,

$$(3.5) \quad \rho_1(X, Y|Z) \leq \rho_{p_n, q_n}(Z) + \Delta_1$$

for some  $\Delta_1$  such that  $E|\Delta_1| < \varepsilon$ . To find such a  $\Delta_1$ , we will first look for a pair  $(f_m, g_m) \in S_0$  such that  $E(f_m g_m|Z) \approx \rho_1(X, Y|Z)$ , and then find  $(f_n^*, g_n^*) \in S_{0, p_n, q_n}$  such that  $(f_n^*, g_n^*) \approx (f_m, g_m)$ . Take

$$(3.6) \quad \Delta_1 = E(f_m g_m|Z) - E(f_n^* g_n^*|Z) + \rho_1(X, Y|Z) - E(f_m g_m|Z),$$

then (3.5) holds and  $E|\Delta_1|$  can be made small if  $m$  and  $n$  are large enough.

To find  $(f_m, g_m) \in S_0$  such that  $E(f_m g_m|Z) \approx \rho_1(X, Y|Z)$ , let  $\{(f_n, g_n)\}_{n=1}^\infty$  be a sequence in  $S_0$  such that  $\{E(f_n g_n|Z)\}$  is an increasing sequence and  $\lim_{n \rightarrow \infty} E(f_n g_n|Z) = \rho_1(X, Y|Z)$ . Let  $\Delta_{2,n} = \rho_1(X, Y|Z) - E(f_n g_n|Z)$ , then  $\lim_{n \rightarrow \infty} E|\Delta_{2,n}| = 0$ , which implies that for every  $\delta > 0$ , there exists  $m$  such that

$$(3.7) \quad E|\Delta_{2,m}| < \delta.$$

To find  $(f_n^*, g_n^*) \in S_{0, p_n, q_n}$  such that  $(f_n^*, g_n^*) \approx (f_m, g_m)$ , note that it follows from (3.1) and (3.2) that for  $n \geq N_0$ , there exists some  $(f_{n,1}, g_{n,1}) \in S_{1, p_n, q_n}$  such that

$$(3.8) \quad \sqrt{E(f_m - f_{n,1})^2} < \delta \quad \text{and} \quad \sqrt{E(g_m - g_{n,1})^2} < \delta.$$

Let  $f_{n,2}(X, Z) = f_{n,1}(X, Z) - E(f_{n,1}|Z)$ ,  $g_{n,2}(Y, Z) = g_{n,1}(Y, Z) - E(g_{n,1}|Z)$ ,

$$f_n^*(X, Z) = \frac{f_{n,2}(X, Z)}{\sqrt{E(f_{n,2}^2|Z)}} I_{(0,\infty)}(E(f_{n,2}^2|Z))$$

and

$$g_n^*(Y, Z) = \frac{g_{n,2}(Y, Z)}{\sqrt{E(g_{n,2}^2|Z)}} I_{(0,\infty)}(E(g_{n,2}^2|Z)),$$

then it follows from (3.3) that  $(f_n^*, g_n^*) \in S_{0, p_n, q_n}$ . To see that  $(f_n^*, g_n^*) \approx (f_m, g_m)$ , let  $\Delta_3 = f_m - f_n^*$  and  $\Delta_4 = g_m - g_n^*$ , then it can be shown that

$$(3.9) \quad E\Delta_3^2 \leq 16\delta^2 + 8\delta$$

and

$$(3.10) \quad E\Delta_4^2 \leq 16\delta^2 + 8\delta.$$

Below we will verify (3.9) only since the verification for (3.10) is similar. Write  $\Delta_3 = f_m - f_{n,2} + f_{n,2} - f_n^*$ , then by (3.8),

$$(3.11) \quad E(f_m - f_{n,2})^2 \leq 4\delta^2$$

since  $E(f_m - f_{n,2})^2 \leq 2(E(f_m - f_{n,1})^2 + E(f_{n,1} - f_{n,2})^2)$  and  $(f_{n,1} - f_{n,2})^2 = (E((f_m - f_{n,1})|Z))^2 \leq E((f_m - f_{n,1})^2|Z)$ . Also,

$$\begin{aligned} E((f_n^* - f_{n,2})^2|Z) &= (1 - \sqrt{E(f_{n,2}^2|Z)})^2 I_{(0,\infty)}(E(f_{n,2}^2|Z)) \\ &\leq |1 - E(f_{n,2}^2|Z)| \\ &= |E((f_m - f_{n,2})^2|Z) - 2E(f_m(f_m - f_{n,2})|Z)| \\ &\leq E((f_m - f_{n,2})^2|Z) + 2\sqrt{E((f_m - f_{n,2})^2|Z)}, \end{aligned}$$

so

$$(3.12) \quad E(f_{n,2} - f_n^*)^2 \leq E(f_m - f_{n,2})^2 + 2\sqrt{E(f_m - f_{n,2})^2} \stackrel{(3.11)}{\leq} 4\delta^2 + 4\delta.$$

Therefore, (3.9) follows from (3.11), (3.12) and the inequality  $E\Delta_3^2 \leq 2(E(f_m - f_{n,2})^2 + E(f_{n,2} - f_n^*)^2)$ .

Finally, the  $\Delta_1$  in (3.6) is  $E(f_n^*\Delta_4|Z) + E(g_n^*\Delta_3|Z) + E(\Delta_3\Delta_4|Z) + \Delta_{2,m}$ , so it follows from (3.9), (3.10), (3.7) and the Cauchy inequality that

$$E|\Delta_1| \leq 3\sqrt{16\delta^2 + 8\delta} + \delta.$$

For  $\varepsilon > 0$ , one can choose  $\delta$  so that  $3\sqrt{16\delta^2 + 8\delta} + \delta < \varepsilon$ , then  $E|\Delta_1| < \varepsilon$  as required. The proof of Fact 2 is complete.  $\square$

Based on Fact 2, it is reasonable to estimate  $\rho_1(X, Y|Z)$  using an estimator for  $\rho_{p,q}(Z)$ , where  $p$  and  $q$  are large. To estimate  $\rho_{p,q}(Z)$ , the following assumption is made:

- (A1) There exists a version of the conditional distribution of  $(X, Y)$  given  $Z$  such that for every bounded function  $g(X, Y)$ ,  $E(g(X, Y)|Z)$  calculated using that version is a continuous function of  $Z$ .

From now on, we will use the version of conditional distribution in (A1) to obtain  $E(g(X, Y)|Z = z)$  for every bounded  $g$  and every  $z$  in the range of  $Z$ . It for each  $(p, q)$ ,  $1 \leq i \leq p$ ,  $1 \leq j \leq q$ ,  $|\phi_{p,i}| \leq 1$  and  $|\psi_{q,j}| \leq 1$ , then each element in  $\Sigma_{\phi,p}(z)$ ,  $\Sigma_{\psi,q}(z)$  and  $\Sigma_{\phi,\psi,p,q}(z)$  is a continuous function of  $z$ , and  $\rho_{p,q}(z)$  is  $\max_{a,b} a^T \Sigma_{\phi,\psi,p,q}(z) b$ , where the maximum is taken over all vectors  $a$  and  $b$  such that

$$a^T \Sigma_{\phi,p}(z) a = 1 = b^T \Sigma_{\psi,q}(z) b.$$

To estimate  $\rho_{p,q}(z)$ , we consider the estimator

$$\hat{\rho}_{p,q}(z) = \max_{a,b} a^T \hat{\Sigma}_{\phi,\psi,p,q}(z) b,$$

where the maximum is taken over all vectors  $a$  and  $b$  such that

$$a^T \hat{\Sigma}_{\phi,p}(z) a = 1 = b^T \hat{\Sigma}_{\psi,q}(z) b,$$

and  $\hat{\Sigma}_{\phi,p}(z)$ ,  $\hat{\Sigma}_{\phi,\psi,p,q}(z)$  and  $\hat{\Sigma}_{\psi,q}(z)$  are obtained by replacing the conditional expectations in  $\Sigma_{\phi,p}(z)$ ,  $\Sigma_{\phi,\psi,p,q}(z)$  and  $\Sigma_{\psi,q}(z)$  by their kernel estimators. Specifically, each element in  $\Sigma_{\phi,p}(z)$ ,  $\Sigma_{\phi,\psi,p,q}(z)$  and  $\Sigma_{\psi,q}(z)$  is of the form  $E(UV|Z=z) - (E(U|Z=z))(E(V|Z=z))$ , where  $U$  and  $V$  are functions of  $X$  or  $Y$ , so each of  $E(UV|Z=z)$ ,  $E(U|Z=z)$  and  $E(V|Z=z)$  is of the form  $E(g(X,Y)|Z=z)$ , which is estimated by

$$(3.13) \quad \hat{E}(g(X,Y)|Z=z) \stackrel{\text{def}}{=} \frac{\sum_{i=1}^n g(X_i, Y_i) k_h(z - Z_i)}{\sum_{i=1}^n k_h(z - Z_i)},$$

where  $k_h(z) = h^{-d} k_0(z/h)$  and  $k_0$  is a kernel function on  $R^d$  satisfying certain conditions which will be specified later. For each  $z \in \mathcal{Z}$ , to make  $\hat{\rho}_{p,q}(z)$  a reasonable estimator for  $\rho_1(X, Y|Z=z)$ , we will take  $p = p_n$ ,  $q = q_n$  and  $h = h_n$ , where  $p_n \rightarrow \infty$ ,  $q_n \rightarrow \infty$  and  $h_n \rightarrow 0$  as  $n \rightarrow \infty$ . The estimator  $\hat{\rho}_{p_n, q_n}(z)$  will be abbreviated as  $\hat{\rho}(z)$  for each  $z \in \mathcal{Z}$ .

The estimator  $\hat{\rho}(z)$  can be expressed in a different form that is easier to analyze. Let  $X_*$  and  $Y_*$  be random vectors of length  $p_n$  and  $q_n$ , respectively, such that given the data  $(X_1, Y_1, Z_1), \dots, (X_n, Y_n, Z_n)$ ,

$$(X_*^T, Y_*^T) = (\phi_{p_n,1}(X_\ell), \dots, \phi_{p_n,p_n}(X_\ell), \psi_{q_n,1}(Y_\ell), \dots, \psi_{q_n,q_n}(Y_\ell))$$

with probability  $k_h(z - Z_\ell) / \sum_{i=1}^n k_h(z - Z_i)$  for  $1 \leq \ell \leq n$ . Then  $\hat{\Sigma}_{\phi,\psi,p,q}(z) = EX_* Y_*^T - EX_* EY_*^T$ ,  $\hat{\Sigma}_{\phi,p}(z) = EX_* X_*^T - EX_* EX_*^T$  and  $\hat{\Sigma}_{\psi,q}(z) = EY_* Y_*^T - EY_* EY_*^T$ , where the expectations are conditional expectations given the data. Therefore, the estimator  $\hat{\rho}(z)$  is the largest canonical coefficient from the centered canonical analysis between  $X_*$  and  $Y_*$ . Note that it follows from (3.3) that

$$(3.14) \quad a_{n,*}^T X_* = 1 = b_{n,*}^T Y_*,$$

where

$$a_{n,*} = (a_{p_n,0,1}, \dots, a_{p_n,0,p_n})^T \quad \text{and} \quad b_{n,*} = (b_{q_n,0,1}, \dots, b_{q_n,0,q_n})^T,$$

so  $\hat{\rho}(z)$  can also be obtained from the noncentered canonical analysis between  $X_*$  and  $Y_*$ . Let

$$V_{1,1}(z) = (E(\phi_{p_n,i}(X)\phi_{p_n,j}(X)|Z=z))_{p_n \times p_n},$$

$$V_{1,2}(z) = (E(\phi_{p_n,i}(X)\psi_{q_n,j}(Y)|Z=z))_{p_n \times q_n},$$

$$V_{2,2}(z) = (E(\psi_{q_n,i}(Y)\psi_{q_n,j}(Y)|Z=z))_{q_n \times q_n} \quad \text{and} \quad V_{2,1}(z) = V_{1,2}(z)^T$$

for  $1 \leq i, j \leq 2$ , let  $\hat{V}_{i,j}(z)$  be the estimator of  $V_{i,j}(z)$  obtained by replacing the conditional expectations in  $V_{i,j}(z)$  by their kernel estimators as in (3.13). Then  $\hat{V}_{1,1}(z) = EX_* X_*^T$ ,  $\hat{V}_{1,2}(z) = EX_* Y_*^T$ ,  $\hat{V}_{2,2}(z) = EY_* Y_*^T$ , so  $\hat{\rho}(z)$  is the square root of the largest eigenvalue of the matrix

$$\hat{V}_{1,2}(z) \hat{V}_{2,2}^{-1}(z) \hat{V}_{2,1}(z) \hat{V}_{1,1}(z)^{-1} - \hat{V}_{1,1}(z) a_{n,*} a_{n,*}^T.$$

Also,  $\rho_{p_n, q_n}(z)$  is the square root of the largest eigenvalue of the matrix

$$V_{1,2}(z)V_{2,2}^{-1}(z)V_{2,1}(z)V_{1,1}(z)^{-1} - V_{1,1}(z)a_{n,*}a_{n,*}^T.$$

To simplify the above matrix expressions, some notation is introduced as follows. For a  $(p_n + q_n) \times (p_n + q_n)$  matrix  $U$ , express  $U$  as

$$\begin{pmatrix} U_{1,1} & U_{1,2} \\ U_{2,1} & U_{2,2} \end{pmatrix},$$

where the dimension of  $U_{1,1}$  is  $p_n \times p_n$ . For  $1 \leq i, j \leq 2$ , let  $g_{i,j}$  be the mapping that maps  $U$  to  $U_{i,j}$ . For a  $p_n \times 1$  vector  $a$  and a  $(p_n + q_n) \times (p_n + q_n)$  matrix  $U$ , define

$$g(U, a) = g_{1,2}(U)g_{2,2}(U)^{-1}g_{2,1}(U)g_{1,1}(U)^{-1} - g_{1,1}(U)aa^T,$$

if  $g_{2,2}(U)$  and  $g_{1,1}(U)$  are invertible. Let

$$V(z) = \begin{pmatrix} V_{1,1}(z) & V_{1,2}(z) \\ V_{2,1}(z) & V_{2,2}(z) \end{pmatrix}$$

and

$$\hat{V}(z) = \begin{pmatrix} \hat{V}_{1,1}(z) & \hat{V}_{1,2}(z) \\ \hat{V}_{2,1}(z) & \hat{V}_{2,2}(z) \end{pmatrix},$$

then  $\hat{\rho}(z)$  is the square root of the largest eigenvalue of  $g(\hat{V}(z), a_{n,*})$  and  $\rho_{p_n, q_n}(z)$  is the square root of the largest eigenvalue of  $g(V(z), a_{n,*})$ .

The matrix  $g(\hat{V}(z), a_{n,*})$  can be replaced by a different matrix if basis change is performed. That is, suppose that

$$\phi = (\phi_{p_n,1}, \dots, \phi_{p_n,p_n})^T \quad \text{and} \quad \psi = (\psi_{q_n,1}, \dots, \psi_{q_n,q_n})^T$$

are replaced by  $\phi^* = P_1\phi$  and  $\psi^* = Q_1\psi$ , respectively, and  $\hat{V}(z)$  becomes  $\hat{V}^*(z)$  after such a change is made. Then  $\hat{\rho}(z)$  is also the square root of the largest eigenvalue of the matrix  $g(\hat{V}^*(z), \alpha^*)$ , where  $\alpha^* = (P_1^{-1})^T a_{n,*}$  is a vector such that  $(\alpha^*)^T \phi^* = 1$ . To make the expression for  $g(V^*(z), \alpha^*)$  simple, the matrices  $P_1$  and  $Q_1$  are chosen so that

$$(3.15) \quad \phi_1^* = 1 = \psi_1^*,$$

$g_{1,1}(V^*(z))$  and  $g_{2,2}(V^*(z))$  are identity matrices, and for  $1 \leq i \leq p_n$  and  $1 \leq j \leq q_n$ ,

$$(3.16) \quad E(\phi_i^*(X)\psi_j^*(Y)|Z=z) = \delta_{i,j}\sqrt{\lambda_i},$$

where  $\phi_i^*$  and  $\psi_j^*$  denote the  $i$ th element in  $\phi^*$  and the  $j$ th element in  $\psi^*$ , respectively,  $\delta_{i,j}$  denotes the Kronecker symbol and the  $\lambda_i$ 's are the eigenvalues of  $g(V^*(z), \alpha^*)$ . Note that  $(\alpha^*)^T = (1, 0, \dots, 0)$  with the above choice of  $P_1$  and  $Q_1$ .

**3.2. Asymptotic properties and a test of conditional independence.** In this section, we will give asymptotic properties of the estimators  $\hat{\rho}(z_k): 1 \leq k \leq n_Z$ , where the  $z_k$ 's are distinct points in  $\mathcal{Z}$ . First, we will establish the consistency of the estimators, which relies on the fact that for each  $k$ , the two matrices  $g(\hat{V}^*(z_k), \alpha^*)$  and  $g(V^*(z_k), \alpha^*)$  are close, and their largest eigenvalues are  $\hat{\rho}^2(z_k)$  and  $\rho_{p_n, q_n}^2(z_k)$ . The difference between  $g(\hat{V}^*(z_k), \alpha^*)$  and  $g(V^*(z_k), \alpha^*)$  depends on the difference of  $\hat{V}^*(z_k)$  and  $V^*(z_k)$ , and the difference between some conditional expectation  $E(g(X, Y, Z)|Z = z)$  and its kernel estimator  $\hat{E}(g(X, Y, Z)|Z = z) = \sum_{i=1}^n w_{0,i}(z)g(X_i, Y_i, z) / \sum_{i=1}^n w_{0,i}(z)$ , where  $w_{0,i}(z) = k_0(h_n^{-1}(z - Z_i))$ . To make it easier to derive the asymptotic properties of  $\hat{E}(g(X, Y, Z)|Z = z)$ , some regularity conditions on the distribution of  $(X, Y, Z)$  are imposed as follows.

- (R1) There exists a  $\sigma$ -finite measure  $\mu$  such that for every  $z \in \mathcal{Z}$ , the conditional distribution of  $(X, Y)$  given  $Z = z$  has a p.d.f.  $f(\cdot|z)$  with respect to  $\mu$ . Also,  $Z$  has a Lebesgue p.d.f.  $f_Z$ , and  $f(x, y|z)$  and  $f_Z(z)$  are twice differentiable with respect to  $z$ .
- (R2) There exists a function  $h$  on  $\mathcal{X} \times \mathcal{Y}$  such that

$$\sup_{z \in \mathcal{Z}} \max \left( |f(x, y|z)|, \max_{1 \leq i \leq d} \left| \frac{\partial}{\partial z_i} f(x, y|z) \right|, \max_{1 \leq i, j \leq d} \left| \frac{\partial^2}{\partial z_i \partial z_j} f(x, y|z) \right| \right) \leq h(x, y)$$

and  $\int h(x, y) d\mu(x, y) < \infty$ .

- (R3) There exist constants  $c_0$  and  $c_1$  such that

$$\sup_{z \in \mathcal{Z}} \max \left( |f_Z(z)|, \max_{1 \leq i \leq d} \left| \frac{\partial}{\partial z_i} f_Z(z) \right|, \max_{1 \leq i, j \leq d} \left| \frac{\partial^2}{\partial z_i \partial z_j} f_Z(z) \right| \right) \leq c_0$$

and  $1/f_Z(z) \leq c_1$  for  $z \in \mathcal{Z}$ .

Note that (R2) implies condition (A1) in Section 3.1. For the kernel function  $k_0$ , conditions (K1) and (K2) are assumed. The notation  $\|\cdot\|$  denotes the Euclidean norm for a vector or the Frobenius norm for a matrix.

- (K1)  $k_0 \geq 0$ ,  $\sup_u k_0(u) < \infty$ ,  $\int k_0(u) du = 1$ ,  $\int u k_0(u) du = 0$  and  $\sigma_0^2 = \int \|u\|^2 k_0(u) du < \infty$ .
- (K2) There exists positive constants  $\gamma_2$  and  $\gamma_3$  that does not depend on  $d$  such that

$$k_0(a) \leq (\gamma_2)^d e^{-\gamma_3 \|a\|^2} \quad \text{for every } a \in R^d.$$

**REMARK.** If  $k_0$  is a product kernel of the form  $k_0(z_1, \dots, z_d) = k_{00}(z_1) \cdots k_{00}(z_d)$ , and

$$k_{00}(x) \leq \gamma_2 e^{-\gamma_3 x^2} \quad \text{for every } x \in R,$$

then condition (K2) holds.

Assume the above conditions, then it is possible to control the difference between  $\hat{V}^*(z_k)$  and  $V^*(z_k)$  using the following result.

LEMMA 1. *Suppose that conditions (R1)–(R3) and (K1)–(K2) hold. Suppose that  $f_{n,1}, \dots, f_{n,k_n}$  are functions defined on  $\mathcal{X} \times \mathcal{Y} \times \mathcal{Z}$ , where  $\mathcal{X}$ ,  $\mathcal{Y}$  and  $\mathcal{Z}$  are the ranges of  $X$ ,  $Y$  and  $Z$ , respectively. Let  $f_Z$  be the p.d.f. of  $Z$ ,  $\hat{f}_Z(z) = (nh_n^d)^{-1} \sum_{i=1}^n k_0(h_n^{-1}(z - Z_i))$  for  $z \in \mathcal{Z}$  and  $c_K = 1/\int k_0^2(s) ds$ . For  $z \in \mathcal{Z}$ , let  $w_i(z) = n^{-1}h_n^{-d}w_{0,i}(z)/\hat{f}_Z(z)$  for  $1 \leq i \leq n$  and*

$$W_{n,j}(z) = \sqrt{nh_n^d c_K f_Z(z)} \left( \left( \sum_{i=1}^n w_i(z) f_{n,j}(X_i, Y_i, z) \right) - E(f_{n,j}(X, Y, z) | Z = z) \right)$$

for  $1 \leq j \leq k_n$ . Suppose that  $\{h_n\}_{n=1}^\infty$  and  $\{\varepsilon_n\}_{n=1}^\infty$  are sequences of positive numbers such that

$$c_{3,1}n^{-\alpha} \leq h_n \leq c_{3,2}n^{-\alpha}$$

for some positive constants  $c_{3,1}$  and  $c_{3,2}$  and  $1/(d+4) < \alpha < 1/d$ , and  $h_n/\varepsilon_n = O(n^{-\beta})$  for some  $\beta > 0$ . Let

$$(3.17) \quad \mathcal{Z}(\varepsilon_n) = \{z \in \mathcal{Z} : \{z' \in R^d : \|z' - z\| < \varepsilon_n\} \subset \mathcal{Z}\}$$

and suppose that  $z_1, \dots, z_{n_Z}$  are points in  $\mathcal{Z}(\varepsilon_n)$  such that

$$(3.18) \quad \|z_k - z_{k^*}\| \geq h_n \quad \text{for } 1 \leq k, k^* \leq n_Z \text{ and } k \neq k^*$$

for large  $n$  and

$$(3.19) \quad \max_{1 \leq k \leq n_Z} \sup_{(x,y) \in \mathcal{X} \times \mathcal{Y}} |f_{n,j}(x, y, z_k)| \leq C_n \quad \text{for some } C_n \geq 1.$$

Suppose that  $k_n n_Z C_n = O((\ln n)^{1/16})$ . Then there exist  $W_{n,1,j,k}$  and  $W_{n,2,j,k} : 1 \leq j \leq k_n, 1 \leq k \leq n_Z$  such that the joint distribution of  $W_{n,1,j,k} + W_{n,2,j,k}$ 's is the same as the joint distribution of  $W_{n,j}(z_k)$ 's,  $\sum_{j=1}^{k_n} \sum_{k=1}^{n_Z} W_{n,2,j,k}^2 = O_P(\exp(-(\ln n)^{1/9}))$ , and  $W_{n,1,j,k}$ 's are jointly normal with  $EW_{n,1,j,k} = 0$  and for  $1 \leq j, \ell \leq k_n$  and  $1 \leq k, k^* \leq n_Z$

$$\begin{aligned} & \text{Cov}(W_{n,1,j,k}, W_{n,1,\ell,k^*}) \\ &= \begin{cases} \text{Cov}(f_{n,j}(X, Y, z_k), f_{n,\ell}(X, Y, z_k) | Z = z_k), & \text{if } k = k^*; \\ 0, & \text{otherwise.} \end{cases} \end{aligned}$$

The proof of Lemma 1 is given in Section 7.1.

The differences between  $\hat{V}^*(z_k)$ 's and  $V^*(z_k)$ 's can be controlled by applying Lemma 1 and taking the  $f_{n,j}(X, Y, z)$ 's to be the functions  $\phi_\ell^*(X)\phi_{\ell'}^*(X)$ ,  $\phi_\ell^*(X)\psi_m^*(Y)$  and  $\psi_m^*(Y)\psi_{m'}^*(Y)$ , where  $1 \leq \ell \leq \ell' \leq p_n$  and  $1 \leq m \leq m' \leq q_n$ . In such case, (3.19) holds under the following conditions.

- (B1) For each  $(p, q)$ ,  $|\phi_{p,k}| \leq 1$  and  $|\psi_{q,\ell}| \leq 1$  for  $1 \leq k \leq p$  and  $1 \leq \ell \leq q$ .  
 (B2) There exists  $\{\delta_n\}$ : a sequence of positive numbers such that for  $1 \leq k \leq n_Z$ , the smallest eigenvalues of the matrices  $V_{1,1}(z_k)$  and  $V_{2,2}(z_k)$  are greater than or equal to  $\delta_n$ .

Under the above conditions, the  $\hat{\rho}(z_k)$ 's are consistent, as stated in Theorem 3.1.

**THEOREM 3.1.** *Suppose that (3.1), (3.2), (3.3), conditions (R1)–(R3), (K1)–(K2) and (B1)–(B2) hold. Suppose that  $\{h_n\}_{n=1}^\infty$  and  $\{\varepsilon_n\}_{n=1}^\infty$  are sequences of positive numbers such that*

$$c_{3,1}n^{-\alpha} \leq h_n \leq c_{3,2}n^{-\alpha}$$

*for some positive constants  $c_{3,1}$  and  $c_{3,2}$  and  $1/(d+4) < \alpha < 1/d$ , and  $h_n/\varepsilon_n = O(n^{-\beta})$  for some  $\beta > 0$ . Suppose that  $z_1, \dots, z_{n_Z}$  are points in  $\mathcal{Z}(\varepsilon_n)$  [defined in (3.17)] such that (3.18) holds and*

$$(3.20) \quad n_Z(p_n + q_n)^2 \max\{1, \delta_n^{-1}(p_n + q_n)\} = O((\ln n)^{1/16}).$$

*Then*

$$(3.21) \quad \sum_{k=1}^{n_Z} (\hat{\rho}^2(z_k) - \rho_{p_n, q_n}^2(z_k))^2 = O_P((nh_n^d)^{-1}(\ln n)^{1/4})$$

*and*

$$(3.22) \quad \left( \sum_{k=1}^{n_Z} \hat{f}_Z(z_k) \hat{\rho}^2(z_k) - \sum_{k=1}^{n_Z} f_Z(z_k) \rho_{p_n, q_n}^2(z_k) \right)^2 = O_P\left(\frac{(\ln n)^{5/16}}{nh_n^d}\right).$$

The proof of Theorem 3.1 is given in Section 7.2.

The next result deals with the asymptotic distribution of  $\sum_{k=1}^{n_Z} \hat{f}_Z(z_k) \hat{\rho}^2(z_k)$  when  $X$  and  $Y$  are conditionally independent given  $Z$ .

**THEOREM 3.2.** *Suppose that the conditions in Theorem 3.1 hold and  $X$  and  $Y$  are conditionally independent given  $Z$ . Then there exist random variables  $\tilde{f}_k$ ,  $\tilde{\rho}^2(z_k)$  and  $\lambda_k : 1 \leq k \leq n_Z$  such that  $\sum_{k=1}^{n_Z} \tilde{f}_k \tilde{\rho}^2(z_k)$  has the same distribution as  $\sum_{k=1}^{n_Z} \hat{f}_Z(z_k) \hat{\rho}^2(z_k)$  and*

$$nh_n^d c_K \sum_{k=1}^{n_Z} \tilde{f}_k \tilde{\rho}^2(z_k) - \sum_{k=1}^{n_Z} \lambda_k = O_P(\exp(-0.5(\ln n)^{1/9})(\ln n)^{3/32}),$$

*where the  $\lambda_k$ 's are independent and each  $\lambda_k$  has the same distribution as the largest eigenvalue of a matrix  $CC^T$ , where  $C$  is a  $(p_n - 1) \times (q_n - 1)$  matrix whose elements are i.i.d.  $N(0, 1)$ .*

The proof of Theorem 3.2 is given in Section 7.3. The result in Theorem 3.2 is similar to that in Lemma 7.2 in [3]. The difference is that the asymptotic result here is derived as the sample size  $n$ ,  $p_n$  and  $q_n$  all tend to  $\infty$ , while in [3], the result is derived as  $n$  tends to  $\infty$ , but  $p_n$  and  $q_n$  are held fixed.

Theorem 3.2 suggests the test that rejects the conditional independence hypothesis at approximate level  $a$  if

$$(3.23) \quad nh_n^d c_K \sum_{k=1}^{n_Z} \hat{f}_Z(z_k) \hat{\rho}^2(z_k) > F_{n_Z, p, q}^{-1}(1-a),$$

where  $F_{n_Z, p, q}$  is the cumulative distribution function of  $\sum_{k=1}^{n_Z} \lambda_k$ .

One can estimate  $F_{n_Z, p, q}^{-1}(1-a)$  in (3.23) using simulated data, but it is also possible to use a normal approximation. Since the  $\lambda_k$ 's are i.i.d., the central limit theorem suggests the asymptotic normality of  $\sum_{k=1}^{n_Z} \lambda_k$  and  $\sum_{k=1}^{n_Z} \hat{f}_Z(z_k) \hat{\rho}^2(z_k)$ . The following corollary gives the conditions that guarantee the asymptotic normality of  $\sum_{k=1}^{n_Z} \hat{f}_Z(z_k) \hat{\rho}^2(z_k)$ .

COROLLARY 1. *Suppose that the conditions in Theorem 3.1 hold*

$$(3.24) \quad \lim_{n \rightarrow \infty} \frac{p_n^3 q_n^3}{\sqrt{n_Z} (\max(p_n, q_n))^{1/3}} = 0$$

and (i) or (ii) holds:

(i)  $q_n = h(p_n)$ , where  $h$  is an increasing function such that  $\lim_{p \rightarrow \infty} h(p)/p$  exists and is greater than or equal to 1.

(ii)  $p_n = h(q_n)$ , where  $h$  is an increasing function such that  $\lim_{q \rightarrow \infty} h(q)/q$  exists and is greater than or equal to 1.

Let  $\mu_{p_n, q_n}$  and  $\sigma_{p_n, q_n}^2$  be the mean and variance of the largest eigenvalue of the matrix  $CC^T$  in Theorem 3.2, respectively, and let the  $\lambda_k$ 's be as in Theorem 3.2, then

$$(3.25) \quad \frac{(\max(p_n, q_n))^{1/6}}{\sigma_{p_n, q_n}} = O(1)$$

and

$$(3.26) \quad \frac{\sum_{k=1}^{n_Z} \lambda_k - n_Z \mu_{p_n, q_n}}{\sqrt{n_Z \sigma_{p_n, q_n}^2}} \xrightarrow{\mathcal{D}} N(0, 1) \quad \text{as } n \rightarrow \infty.$$

If  $X$  and  $Y$  are conditionally independent given  $Z$ , then

$$(3.27) \quad \frac{nh_n^d c_K \sum_{k=1}^{n_Z} \hat{f}_Z(z_k) \hat{\rho}^2(z_k) - n_Z \mu_{p_n, q_n}}{\sqrt{n_Z \sigma_{p_n, q_n}^2}} \xrightarrow{\mathcal{D}} N(0, 1) \quad \text{as } n \rightarrow \infty.$$



The proof of Corollary 1 is given in Section 7.4. Corollary 1 gives the test that rejects the conditional independence hypothesis if

$$(3.28) \quad \frac{nh_n^d c_K \sum_{k=1}^{n_Z} \hat{f}_Z(z_k) \hat{\rho}^2(z_k) - n_Z \mu_{p_n, q_n}}{\sqrt{n_Z \sigma_{p_n, q_n}^2}} \geq \Phi^{-1}(1-a),$$

where  $\Phi$  is the cumulative distribution function for the standard normal distribution. Here,  $\mu_{p_n, q_n}$  and  $\sigma_{p_n, q_n}^2$  can be approximated by the sample mean and variance of a random sample from the distribution of the largest eigenvalue of the matrix  $CC^T$ .

To distinguish the two tests mentioned above, we will refer to the test with rejection region in (3.28) as test 1N and the test with rejection region in (3.23) as test 1. Note that under the conditions in Corollary 1, test 1 does not differ from test 1N much since the rejection region for test 1 can be written as

$$\frac{nh_n^d c_K \sum_{k=1}^{n_Z} \hat{f}_Z(z_k) \hat{\rho}^2(z_k) - n_Z \mu_{p_n, q_n}}{\sqrt{n_Z \sigma_{p_n, q_n}^2}} \geq I + \Phi^{-1}(1-a),$$

where

$$(3.29) \quad I = \frac{F_{n_Z, p, q}^{-1}(1-a) - n_Z \mu_{p_n, q_n}}{\sqrt{n_Z \sigma_{p_n, q_n}^2}} - \Phi^{-1}(1-a) = o(1)$$

by (3.26). Therefore, both tests 1 and 1N are of asymptotic significance level  $a$ . Below we will discuss the consistency and asymptotic power of test 1N only since the same properties of test 1 can be established similarly using (3.29).

Suppose all the conditions in Theorem 3.1 hold, then test that 1N is also consistent if the  $z_k$ 's are chosen in a way such that there exist a constant  $c_3 > 0$  and a sequence  $\{\eta_{1,n}\}_{n=1}^{\infty}$  such that  $\eta_{1,n} > 0$  for every  $n$ ,  $\lim_{n \rightarrow \infty} \eta_{1,n} = 0$  and

$$(3.30) \quad \frac{1}{n_Z} \sum_{k=1}^{n_Z} f_Z(z_k) \rho_{p_n, q_n}^2(z_k) - c_3 E \rho_{p_n, q_n}^2(Z) = o_P(\eta_{1,n}).$$

To see that test 1N is consistent, note that  $0 \leq \mu_{p_n, q_n} \leq E \operatorname{tr}(CC^T)$  and  $\sigma_{p_n, q_n}^2 \leq E(\operatorname{tr}(CC^T))^2$ , where  $CC^T$  is as in Theorem 3.2. Therefore,  $\mu_{p_n, q_n} = O(p_n q_n)$  and  $\sigma_{p_n, q_n}^2 = O(p_n^2 q_n^2)$ . Then it follows from (3.22), (3.30) and Fact 2 that  $n_Z^{-1} \sum_{k=1}^{n_Z} \hat{f}_Z(z_k) \hat{\rho}^2(z_k) - c_3 E \rho_1^2(X, Y|Z) = O_P((\ln n)^{5/32} / n_Z \sqrt{nh_n^d}) + o_P(\eta_{1,n}) + c_3 E \rho_{p_n, q_n}^2(Z) - c_3 E \rho_1^2(X, Y|Z) = o_P(1)$ , so

$$\frac{nh_n^d c_K \sum_{k=1}^{n_Z} \hat{f}_Z(z_k) \hat{\rho}^2(z_k) - n_Z \mu_{p_n, q_n}}{\sqrt{n_Z \sigma_{p_n, q_n}^2}}$$

$$\geq \frac{\sqrt{n_Z}(nh_n^d c_K(c_3 E\rho_1^2(X, Y|Z) + o_P(1)) + O(p_n q_n))}{c_{2,1} p_n q_n},$$

where  $c_{2,1} > 0$  is a constant. Thus, the left-hand side in (3.28) tends to  $\infty$  as  $n \rightarrow \infty$  when  $E\rho_1^2(X, Y|Z) > 0$ , which implies that the probability that (3.28) holds tends to 1 if  $X$  and  $Y$  are not conditionally independent given  $Z$ .

Test 1N can also reject an alternative where  $E\rho_{p_n, q_n}^2(Z)$  is small under the conditions in Theorem 3.1. Indeed, for  $\{\eta_{1,n}\}_{n=1}^\infty$  such that  $\eta_{1,n} > 0$  for every  $n$ ,  $\lim_{n \rightarrow \infty} \eta_{1,n} = 0$  and (3.30) holds, if

$$(3.31) \quad \frac{\max(\eta_{1,n}, (\ln n)^{5/32}/(n_Z \sqrt{nh_n^d}))}{E\rho_{p_n, q_n}^2(Z)} = o(1),$$

then the probability that (3.28) holds tends to 1 since

$$\begin{aligned} & \frac{nh_n^d c_K \sum_{k=1}^{n_Z} \hat{f}_Z(z_k) \hat{\rho}^2(z_k) - n_Z \mu_{p_n, q_n}}{\sqrt{n_Z \sigma_{p_n, q_n}^2}} \\ & \geq \left( \sqrt{n_Z} \left( nh_n^d c_K \left( c_3 E\rho_{p_n, q_n}^2(Z) \right. \right. \right. \\ & \quad \left. \left. \left. + O_P\left( \frac{(\ln n)^{5/32}}{n_Z \sqrt{nh_n^d}} \right) + o_P(\eta_{1,n}) \right) + O(p_n q_n) \right) \right) \\ & \quad \times (c_{2,1} p_n q_n)^{-1}, \end{aligned}$$

where  $p_n q_n / (nh_n^d E\rho_{p_n, q_n}^2(Z)) = O((\ln n)^{1/16} / (n_Z nh_n^d E\rho_{p_n, q_n}^2(Z))) = o(1)$  by (3.20) and (3.31), and  $p_n q_n / (\sqrt{n_Z} nh_n^d E\rho_{p_n, q_n}^2(Z)) = o(1)$ . In summary, test 1N can reject an alternative where  $E\rho_{p_n, q_n}^2(Z)$  tends to zero at a rate that is slower than  $\max(\eta_{1,n}, (\ln n)^{5/32}/(n_Z \sqrt{nh_n^d}))$ , where  $\eta_{1,n}$  is determined by (3.30). An example that satisfies (3.30) and the conditions in Corollary 1 will be given in Section 4. In that example,  $\eta_{1,n} = p_n^{11} n_Z^{-1/d}$ .

**4. An example.** In this section, an example is given to illustrate the verification of the conditions in Corollary 1, assuming (R1)–(R3) and the condition that there exists a positive constant  $c_{1,1}$  such that

$$(4.1) \quad f_{X|Z}(x|z) \geq c_{1,1} \quad \text{and} \quad f_{Y|Z}(y|z) \geq c_{1,1} \\ \text{for all } (x, y, z) \in \mathcal{X} \times \mathcal{Y} \times \mathcal{Z},$$

where  $f_{X|Z}(\cdot|z)$  and  $f_{Y|Z}(\cdot|z)$  are conditional probability densities of  $X$  and  $Y$ , respectively, given  $Z = z$ , with respect to Lebesgue measures.

EXAMPLE 1. Suppose that  $X$ ,  $Y$  and  $Z$  are random vectors that take values in  $[0, 1]^{d_x}$ ,  $[0, 1]^{d_y}$  and  $[0, 1]^d$ , respectively. Suppose that (R1)–(R3), and (4.1) hold. Choose the basis functions as follows. Let  $\Lambda$  be the set of all positive integers and  $\Lambda(k) = \{m^k : m \in \Lambda\}$  for  $k \in \Lambda$ . For  $k, i_1, \dots, i_k \in \Lambda$  and  $h_0 > 0$ , let

$$h_{k,h_0,i_1,\dots,i_k}(x_1, \dots, x_k) = \prod_{j=1}^k I_{A_{i_j,h_0}}(x_j) \quad \text{for } (x_1, \dots, x_k) \in [0, 1]^k,$$

where

$$A_{i_j,h_0} = \begin{cases} (h_0(i_j - 1), h_0 i_j], & \text{if } i_j > 1; \\ [h_0(i_j - 1), h_0 i_j], & \text{if } i_j = 1. \end{cases}$$

For  $p, q, r \in \Lambda$ , let

$$\{\phi_{p,i} : 1 \leq i \leq p\} = \{h_{d_x, p^{-1/d_x}, i_1, \dots, i_{d_x}} : 1 \leq i_1, \dots, i_{d_x} \leq p^{1/d_x}\},$$

$$\{\psi_{q,j} : 1 \leq j \leq q\} = \{h_{d_y, q^{-1/d_y}, i_1, \dots, i_{d_y}} : 1 \leq i_1, \dots, i_{d_y} \leq q^{1/d_y}\}$$

and

$$\{\theta_{r,k} : 1 \leq k \leq r\} = \{h_{d, r^{-1/d}, i_1, \dots, i_d} : 1 \leq i_1, \dots, i_d \leq r^{1/d}\}.$$

Take  $k_0$  to be the product kernel function such that

$$k_0(z_1, \dots, z_d) = k_{00}(z_1) \cdots k_{00}(z_d),$$

where  $k_{00}$  is the probability density function for the standard normal distribution. Let  $h_n = n^{-a}$ , where  $1/(d+4) < a < 1/d$ . Let  $n_Z^*$  to be the largest number in  $\Lambda(d)$  such that  $n_Z^* \leq (\ln n)^{1/32}$ , and let

$$\{z_k : 1 \leq k \leq n_Z\} = \left\{ \left( \frac{i_1}{(n_Z^*)^{1/d}}, \dots, \frac{i_d}{(n_Z^*)^{1/d}} \right) : 1 \leq i_1, \dots, i_d < (n_Z^*)^{1/d} \right\},$$

so  $n_Z = ((n_Z^*)^{1/d} - 1)^d$ . Suppose that  $\{p_n\}$  is a sequence in  $\Lambda(d_x) \cap \Lambda(d_y)$  such that  $\lim_{n \rightarrow \infty} p_n = \infty$  and  $q_n = p_n$ . If

$$(4.2) \quad p_n^{12} \leq n_Z,$$

then all the conditions in Corollary 1 hold. If

$$(4.3) \quad p_n^{12} \leq n_Z^{1/d},$$

then (3.30) holds with  $\eta_{1,n} = p_n^{11} n_Z^{-1/d}$ .

PROOF. We will first show that all the conditions in Corollary 1 hold assuming (4.2). It is clear that (3.1), (3.2) and (3.3), and conditions (B1), (K1) and (K2) hold.

To find the  $\delta_n$  in condition (B2), note that for  $z \in \mathcal{Z}$ , the smallest eigenvalue of  $V_{1,1}(z)$  is the minimum of  $\{E(\phi_{p_n,i}(X)|Z=z): 1 \leq i \leq p_n\}$ , which is the minimum of  $\{E(h_{d_x, p_n^{-1/d_x}, i_1, \dots, i_{d_x}}(X)|Z=z): 1 \leq i_1, \dots, i_{d_x} \leq p_n^{1/d_x}\}$ . Under (4.1), for  $m \in \Lambda$  and  $1 \leq i_1, \dots, i_{d_x} \leq m$ ,

$$\begin{aligned} & E(h_{d_x, 1/m, i_1, \dots, i_{d_x}}(X)|Z=z) \\ &= \int_{(i_1-1)/m}^{i_1/m} \cdots \int_{(i_{d_x}-1)/m}^{i_{d_x}/m} f_{X|Z}(x_1, \dots, x_{d_x}|z) dx_{d_x} \cdots dx_1 \geq \frac{c_{1,1}}{m^{d_x}}. \end{aligned}$$

Take  $m = p_n^{1/d_x}$ , and we have that the smallest eigenvalue of  $V_{1,1}(z)$  is at least  $c_{1,1}/p_n$ . Similarly,  $c_{1,1}/p_n$  is also a lower bound for the smallest eigenvalue of  $V_{2,2}(z)$  and (B2) holds with  $\delta_n = c_{1,1}/p_n$ . Furthermore, (3.20) holds since

$$n_Z(p_n + q_n)^2 \max\{1, \delta_n^{-1}(p_n + q_n)\} = O(n_Z p_n^4) = O(n_Z^2).$$

Finally, the  $z_k$ 's are in  $\mathcal{Z}(\varepsilon_n)$  with  $\varepsilon_n = (n_Z^*)^{-1/d}$  and  $h_n/\varepsilon_n = O(n^{-\beta})$  for  $0 < \beta < \alpha$ . For  $1 \leq k, k^* \leq n_Z$ , and  $k \neq k^*$ ,  $\|z_k - z_{k^*}\| \geq (n_Z^*)^{-1/d} \geq n^{-a}$ , so (3.18) holds. Also, (3.24) holds since

$$\frac{p_n^3 q_n^3}{\sqrt{n_Z}(\max(p_n, q_n))^{1/3}} = p_n^{-1/3} \sqrt{\frac{p_n^{12}}{n_Z}} = o(1).$$

Therefore, all the conditions in Corollary 1 hold for this example.

The verification of (3.30) is based on the fact that there exist positive constants  $c_{4,1}$  and  $\eta_0$  such that

$$(4.4) \quad |\rho_{p_n, q_n}^2(z) - \rho_{p_n, q_n}^2(z')| \leq c_{4,1} p_n^{11} \|z - z'\| \quad \text{if } p_n^3 \|z - z'\| < \eta_0.$$

Below we will first check (3.30) assuming that (4.4) holds and then prove (4.4). Suppose that (4.3) holds. Let  $g_n(z) = f_Z(z) \rho_{p_n, q_n}^2(z)$ . Since  $f_Z$  is Lipschitz continuous, (4.4) implies that there exists a constant  $c_{4,2} > 0$  such that

$$|g_n(z) - g_n(z')| \leq c_{4,2} p_n^{11} \|z - z'\| \quad \text{if } p_n^3 \|z - z'\| < \eta_0.$$

Let  $\{z_{1+n_Z}, \dots, z_{n_Z^*}\}$  be the set

$$\left\{ \left( \frac{i_1}{(n_Z^*)^{1/d}}, \dots, \frac{i_d}{(n_Z^*)^{1/d}} \right) : 1 \leq i_1, \dots, i_d \leq (n_Z^*)^{1/d} \right\} \cap \{z_k : 1 \leq k \leq n_Z\}^c,$$

then

$$\left| \sum_{k=1}^{n_Z^*} g_n(z_k) \left( \frac{1}{(n_Z^*)^{1/d}} \right)^d - \int_{\mathcal{Z}} g_n(z) dz \right| \leq 2c_{4,2} p_n^{11} \sqrt{d} \left( \frac{1}{n_Z^*} \right)^{1/d},$$

if  $p_n^3(n_Z^*)^{-1/d} < \eta_0$ . Since  $|g_n(z)| \leq c_0$  by (R3) and there exists a positive constant  $c_{4,3}$  depending on  $d$  such that

$$n_Z^* - n_Z \begin{cases} \leq c_{4,3}(n_Z^*)^{1/d}, & \text{if } d \geq 2; \\ = 1, & \text{if } d = 1, \end{cases}$$

we have

$$\begin{aligned} & \left| n_Z^{-1} \sum_{k=1}^{n_Z} f_Z(z_k) \rho_{p_n, q_n}^2(z_k) - \frac{\int_{\mathcal{Z}} f_Z(z) \rho_{p_n, q_n}^2(z) dz}{\int_{\mathcal{Z}} 1 dz} \right| \\ &= \left| \frac{n_Z^*}{n_Z} \left( \frac{1}{n_Z^*} \sum_{k=1}^{n_Z^*} g_n(z_k) - \int_{\mathcal{Z}} g_n(z) dz \right) \right. \\ & \quad \left. - \frac{\sum_{k=1+n_Z}^{n_Z^*} g_n(z_k)}{n_Z} + \left( \frac{n_Z^*}{n_Z} - 1 \right) \int_{\mathcal{Z}} g_n(z) dz \right| \\ &\leq \frac{n_Z^*}{n_Z} \left| \frac{1}{n_Z^*} \sum_{k=1}^{n_Z^*} g_n(z_k) - \int_{\mathcal{Z}} g_n(z) dz \right| + c_0 \left( 1 + \int_{\mathcal{Z}} 1 dz \right) \left( \frac{n_Z^* - n_Z}{n_Z} \right) \\ &\leq \frac{c_{4,4} p_n^{11}}{n_Z^{1/d}} \end{aligned}$$

for some constant  $c_{4,4} > 0$  if  $p_n^3(n_Z^*)^{-1/d} < \eta_0$ . Since  $p_n^{12} \leq n_Z^{1/d}$ ,  $p_n^3 n_Z^{-1/d} = o(1)$ , so

$$\left| n_Z^{-1} \sum_{k=1}^{n_Z} f_Z(z_k) \rho_{p_n, q_n}^2(z_k) - \frac{\int_{\mathcal{Z}} f_Z(z) \rho_{p_n, q_n}^2(z) dz}{\int_{\mathcal{Z}} 1 dz} \right| = O_P\left(\frac{p_n^{11}}{n_Z^{1/d}}\right)$$

and  $p_n^{11} n_Z^{-1/d} = o(1)$ . Take  $\eta_{1,n} = p_n^{11} n_Z^{-1/d}$  and  $c_3 = (\int_{\mathcal{Z}} 1 dz)^{-1} = 1$ , then (3.30) holds.

It remains to prove (4.4). Recall that for  $z \in \mathcal{Z}$ ,  $\rho_{p_n, q_n}^2(z)$  is the largest eigenvalue of  $g(V(z), a_{n,*})$ , as mentioned in Section 3.1. Thus,  $|\rho_{p_n, q_n}^2(z) - \rho_{p_n, q_n}^2(z')|$  is bounded by  $\|g(V(z), a_{n,*}) - g(V(z'), a_{n,*})\|$ . For  $1 \leq i, j \leq 2$ , let  $g_{i,j}^*$  be as defined in (7.8) and let  $\Delta_{i,j} = g_{i,j}^*(V(z')) - g_{i,j}^*(V(z))$  for  $1 \leq i, j \leq 2$ , then from the fact that  $\|AB\| \leq \|A\| \|B\|$  for two matrices  $A$  and  $B$ , we have

$$\begin{aligned} & \|g(V(z), a_{n,*}) - g(V(z'), a_{n,*})\| \\ (4.5) \quad & \leq \prod_{i=1}^2 \prod_{j=1}^2 (\|g_{i,j}^*(V(z))\| + \|\Delta_{i,j}\|) - \prod_{i=1}^2 \prod_{j=1}^2 \|g_{i,j}^*(V(z))\| \\ & \quad + \|g_{1,1}(V(z')) - g_{1,1}(V(z))\| \|a_{n,*}\|^2. \end{aligned}$$

The bounds for the  $\|g_{i,j}^*(V(z))\|$ 's are derived as follows. Since the elements in  $V(z)$  are bounded by 1 and the smallest eigenvalue of  $g_{i,i}(V(z))$  is at least  $c_{1,1}/p_n$  for  $1 \leq i \leq 2$ , we have

$$\max(\|g_{1,2}^*(V(z))\|, \|g_{2,1}^*(V(z))\|) \leq p_n,$$

$$\|g_{1,1}^*(V(z))\|^2 \leq \frac{p_n^2}{(c_{1,1}/p_n)^2} = \frac{p_n^4}{c_{1,1}^2}$$

and

$$\|g_{2,2}^*(V(z))\| \leq \frac{p_n^2}{c_{1,1}}.$$

To find bounds for  $\|g_{1,1}(V(z')) - g_{1,1}(V(z))\|$  and  $\|\Delta_{i,j}\|$ 's, note that from (R3), each element in  $g_{i,j}(V(z')) - g_{i,j}(V(z))$  is bounded by  $\sqrt{d} \int h(x, y) d\mu(x, y) \|z - z'\|$ , so

$$\begin{aligned} & \max(\|\Delta_{1,2}\|, \|\Delta_{2,1}\|, \|g_{1,1}(V(z')) - g_{1,1}(V(z))\|) \\ & \leq p_n \sqrt{d} \int h(x, y) d\mu(x, y) \|z - z'\|. \end{aligned}$$

For  $1 \leq i \leq 2$ , by Fact 4,

$$\|\Delta_{i,i}\| \leq \frac{\|g_{i,i}^*(V(z))\|^2 \|g_{i,i}(V(z')) - g_{i,i}(V(z))\|}{1 - \|g_{i,i}^*(V(z))\| \|g_{i,i}(V(z')) - g_{i,i}(V(z))\|},$$

if  $\|g_{i,i}^*(V(z))\| \|g_{i,i}(V(z')) - g_{i,i}(V(z))\| < 1$ , so

$$\|\Delta_{i,i}\| \leq \frac{2\sqrt{d}p_n^5}{c_{1,1}^2} \int h(x, y) d\mu(x, y) \|z - z'\|,$$

if

$$(4.6) \quad \frac{\sqrt{d}p_n^3}{c_{1,1}} \int h(x, y) d\mu(x, y) \|z - z'\| < \frac{1}{2}.$$

To give a bound for  $\|a_{n,*}\|$ , note that the smallest eigenvalue of  $g_{1,1}(V(z))$  is at least  $c_{1,1}/p_n$  and at most

$$\frac{a_{n,*}^T g_{1,1}(V(z)) a_{n,*}}{a_{n,*}^T a_{n,*}} = \frac{1}{\|a_{n,*}\|^2},$$

so

$$\|a_{n,*}\| \leq \sqrt{\frac{p_n}{c_{1,1}}}.$$

From (4.5) and the above bounds for  $\|a_{n,*}\|$ , the  $\|g_{i,j}^*(V(z))\|$ 's and  $\|\Delta_{i,j}\|$ 's, we have

$$\|g(V(z), a_{n,*}) - g(V(z'), a_{n,*})\| \leq c_{4,1} p_n^{11} \|z - z'\|$$

for some constant  $c_{4,1}$  if (4.6) holds. Therefore, (4.4) holds and the proof for the results in Example 1 is complete.  $\square$

**5. Simulation studies.** In this section, results of several simulation experiments are presented. Those experiments are designed to demonstrate the performance of test 1 introduced in Section 3.2.

In Section 3.2, test 1N is also introduced, but no simulation studies are done for it in this section. The reason is as follows. Test 1N is constructed based on the normal approximation for  $\sum_{k=1}^{n_Z} \lambda_k$ . Using the parameter set-up in Table 2, the selected  $n_Z$  is only 4 or 5 and the normal approximation for  $\sum_{k=1}^{n_Z} \lambda_k$  is not expected to work well.

For simplicity, in all the simulation experiments here,  $X, Y, Z$  are one dimensional and only the following distributions for  $(X, Y, Z)$  are considered.

- (M1)  $(X, Y) = (\Phi(Z\epsilon_1), \Phi(Z\epsilon_2))$ , where  $\epsilon_1, \epsilon_2$  and  $Z$  are independent,  $Z$  follows the uniform distribution on  $[0, 1]$ , and  $\epsilon_i$  follows the standard normal distribution for  $i = 1, 2$ .
- (M2)  $Z$  follows the standard normal distribution, and the conditional distribution of  $(X, Y)$  given  $Z = z$  is bivariate normal with mean  $\mu$  and covariance matrix  $\Sigma$ , where

$$(5.1) \quad \mu = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \quad \Sigma = \begin{pmatrix} 1 & \rho(z) \\ \rho(z) & 1 \end{pmatrix}$$

and the  $\rho(z)$  in (5.1) is taken to be  $a(|1 - 2\Phi(z)|)$  with  $a \in \{0, 0.1, 0.3\}$ .

- (M3)  $(X, Y, Z) = (\Phi(X_0), \Phi(Y_0), \Phi(Z_0))$ , where  $Z_0$  follows the  $t$ -distribution with degree of freedom 1, and the conditional distribution of  $(X_0, Y_0)$  given  $\Phi(Z_0) = z$  is bivariate normal with mean  $\mu$  and covariance matrix  $\Sigma$ , where  $\mu$  and  $\Sigma$  are as in (5.1) and the  $\rho(z)$  in (5.1) is taken to be  $a(|1 - 2z|)$  with  $a \in \{0, 0.1, 0.3\}$ .

Here, (M1) is used for parameter selection and (M2) and (M3) are used for checking the power of test 1. In (M1),  $X$  and  $Y$  are conditionally independent given  $Z$ . In (M2) and (M3),  $\rho_1(X, Y|Z = z) = \rho(z)$  and  $E\rho_1(X, Y|Z)$  is proportional to  $a$ .

The details of parameter selection are given in Section 5.1 and the experimental results are given in Section 5.2.

5.1. *Parameter selection.* To apply test 1, certain parameters need to be chosen, including the kernel function  $k_0$ , the kernel bandwidth  $h_n$ , the basis functions  $\phi_{p_n,i}$ 's and  $\psi_{q_n,j}$ 's and the evaluation points  $z_k$ 's, which are chosen as follows.

(S1)  $k_0$  and the basis functions  $\phi_{p,i}$ 's and  $\psi_{q,j}$ 's are chosen as in Example 1 in Section 4 with  $p_n = q_n = 2$ . Since the basis functions are supported on  $[0, 1]$ , if  $X$ ,  $Y$  and  $Z$  do not take values in  $[0, 1]$  [such as in (M2)], then the data  $\{(X_i, Y_i, Z_i)\}_{i=1}^n$  will be transformed to  $\{(\Phi(X_i), \Phi(Y_i), \Phi(Z_i))\}_{i=1}^n$  before applying test 1. The bandwidth  $h_n$  is chosen to be the  $h$  that minimizes

$$(5.2) \quad \int_{0.143h^{0.121}}^{1-0.143h^{0.121}} E(\hat{f}_Z(z) - 1)^2 dz$$

over  $(0, 0.5]$ , where  $\hat{f}_Z$  is the kernel density estimator based on a sample of size  $n$  from the uniform distribution on  $[0, 1]$  with kernel  $k_0$  and bandwidth  $h$ . Below are the  $h_n$ 's used for different  $n$ 's.

The  $z_k$ 's are points in  $I_n = [0.143h_n^{0.121}, 1 - 0.143h_n^{0.121}]$  such that  $z_k = 0.143h_n^{0.121} + (k-1)h_{0,n}$ , where  $h_{0,n}$  is a given positive number. Here, the  $\varepsilon_n$  is taken to be  $0.143h_n^{0.121}$ , so the  $z_k$ 's are chosen so that they are  $0.143h_n^{0.121}$  away from the boundary and the integral in (5.2) is over  $[0.143h^{0.121}, 1 - 0.143h^{0.121}]$ .

With the parameter set-up in (S1), it remains to choose  $h_{0,n}$ . The  $h_{0,n}$  is chosen to be the smallest multiple of 0.01 such that the distribution for the test 1 statistic  $nh_n^d c_K \sum_{k=1}^{n_Z} \hat{f}_k \hat{\rho}^2(z_k)$  based on 1000 samples of size  $n$  from (M1) is similar to the distribution of  $\sum_{k=1}^{n_Z} \lambda_k$  ( $\chi^2$  with  $n_Z$  degrees of freedom), as stated in Theorem 3.2. The one-sample Kolmogorov–Smirnov test is used to determine whether the two distributions are similar. Below are the  $h_{0,n}$ 's used for  $n = 10,000$  and  $n = 5000$ .

For the above procedure for selecting  $h_{0,n}$ , when  $n = 500$  or  $n = 1000$ , it seems that the distribution of  $nh_n^d c_K \sum_{k=1}^{n_Z} \hat{f}_k \hat{\rho}^2(z_k)$  cannot be approximated well by the distribution of  $\sum_{k=1}^{n_Z} \lambda_k$ , regardless what  $h_{0,n}$  is used. To overcome this problem, one may use local bootstrap to determine the rejection region.

The idea of using local bootstrap is to draw samples  $\{(X_i^*, Y_i^*, Z_i^*)\}_{i=1}^n$  from the distribution of  $(X^*, Y^*, Z^*)$ , where  $Z^*$ 's distribution is close to the distribution of  $Z$  and the conditional distributions of  $X^*$  given  $Z^* = z$  and  $Y^*$  given  $Z^* = z$  are close to the conditional distributions of  $X$  given  $Z = z$  and  $Y$  given  $Z = z$ , yet  $X^*$  and  $Y^*$  are conditionally independent given  $Z^*$ . Therefore, if  $X$  and  $Y$  are conditionally independent given  $Z$ , then the local bootstrap resamples  $\{(X_i^*, Y_i^*, Z_i^*)\}_{i=1}^n$  should behave like a random sample from  $(X, Y, Z)$ . One can then compute the test 1 statistic



TABLE 1  
Selected  $h_n$  's for different  $n$  's

$n$	10,000	5000	1000	500
$h_n$	0.05935281	0.06525282	0.08533451	0.0983018

$nh_n^d c_K \sum_{k=1}^{n_Z} \hat{f}_k \hat{\rho}^2(z_k)$  for the original sample and for each local bootstrap resample. If the statistic computed based on the original sample is larger than  $(1-a)\%$  of the statistics computed based on the local bootstrap resamples, then the conditional independence hypothesis is rejected at level  $a$ .

The local bootstrap procedure used here is the same as the one proposed by Paparoditis and Politis [8] except that here the  $Z_i$ 's are not lagged variables. For a given sample  $\{(X_i, Y_i, Z_i)\}_{i=1}^n$ , a local bootstrap resample  $\{(X_i^*, Y_i^*, Z_i^*)\}_{i=1}^n$  is generated as follows.

- Step 1. Draw a random sample  $(Z_1^*, \dots, Z_n^*)$  from the empirical cumulative distribution function  $\hat{F}_Z$ , where

$$\hat{F}_Z(z) = \frac{1}{n} \sum_{i=1}^n I_{(-\infty, Z_i]}(z).$$

- Step 2. For  $1 \leq i \leq n$ , for each  $Z_i^*$  from Step 1, draw  $X_i^*$  and  $Y_i^*$  independently from the empirical conditional cumulative distribution functions  $\hat{F}_{X|Z=Z_i^*}$  and  $\hat{F}_{Y|Z=Z_i^*}$ , respectively, where

$$\hat{F}_{X|Z=Z_i^*}(x) = \frac{\sum_{i=1}^n k_0((Z_i^* - Z_i)/b) I_{(-\infty, X_i]}(x)}{\sum_{i=1}^n k_0((Z_i^* - Z_i)/b)}$$

and

$$\hat{F}_{Y|Z=Z_i^*}(y) = \frac{\sum_{i=1}^n k_0((Z_i^* - Z_i)/b) I_{(-\infty, Y_i]}(y)}{\sum_{i=1}^n k_0((Z_i^* - Z_i)/b)}.$$

The parameters for test 1 with local bootstrap are chosen as follows. The bandwidth  $b$  is taken to be  $h_n^{0.4}$ ,  $p_n = q_n = 2$  and  $h_{0,n} = 0.4$ , where  $h_n$  is as in Table 1.

TABLE 2  
 $h_{0,n}$  's for different  $n$  's

$n$	10,000	5000
$h_{0,n}$	0.16	0.2

5.2. *Experiments.* The objective of the first experiment is to compare the power of test 1 with that of a Hellinger distance-based test proposed by Su and White [13]. The critical value for Su and White's test can be determined using the asymptotic distribution of the test statistic or using local bootstrap. To distinguish between the two cases, we use test 2A to denote the asymptotic distribution-based version of Su and White's test and test 2B to denote the local bootstrap version. While test 2B is recommended by Su and White [13], test 2A is used here to save time for computation.

In this experiment, both tests 1 and 2A are carried out for 1000 random samples of size  $n = 10^4$ , where the distribution of  $(X, Y, Z)$  is as in (M2) or (M3). Under (M2), test 1 is applied to transformed data, as mentioned in Section 5.1. Test 2A is applied to normalized data and the bandwidth parameter in the kernel estimators in the test statistic is taken to be  $n^{-1/8.5}$ , as in [13]. The power estimates based on data from (M2) and (M3) with  $n = 10^4$  are given in Table 3. The asymptotic significance level is 0.05. It is shown in Table 3 that power estimates for test 1 when  $a = 0$  and  $a = 0.1$  are larger than those for test 2A.

To explore the power performance of test 2B without actually running the local bootstrap procedure, approximate critical values for test 2B under (M2) and (M3) are used. To obtain these approximate critical values, note that under (M2) or (M3), for large  $n$ , a local bootstrap resample for  $a = 0.1$  or  $a = 0.3$  is approximately distributed as a random sample for the  $a = 0$  case, so the critical value for test 2B can be approximated by the 95% sample quantile of the 1000 test 2A statistics from the first experiment for the  $a = 0$  case. Then the power estimates for test 2B can be approximated by the proportions of the 1000 test 2A statistics from the first experiment under different alternatives that exceed the approximate critical values. The approximate power estimates are given in Table 4. Note that the approximate power estimates for test 2B are often larger than the power estimates for test 2A in Table 3, which suggests that test 2B is more powerful than test 2A.

To investigate the performance of test 1 when the sample size is smaller, in the next experiment, power estimates for test 1 are computed based on 1000 random samples of size  $n = 5000$  from (M2) and (M3). The results are

TABLE 3  
Power comparison between tests 1 and 2A

	$a = 0$		$a = 0.1$		$a = 0.3$	
	Test 1	Test 2A	Test 1	Test 2A	Test 1	Test 2A
(M2)	0.049	0.028	0.65	0.076	1	0.95
(M3)	0.041	0.029	0.572	0.119	1	1

TABLE 4  
Approximated power estimates for test 2B

	$a = 0.1$	$a = 0.3$
(M2)	0.128	0.971
(M3)	0.241	1

given in Table 5. The results for  $n = 10^4$  from the first experiment are also included for comparison. The asymptotic significance level is 0.05 as before. Table 5 shows that test 1 is more powerful when  $n$  is larger.

Finally, for smaller sample size such as  $n = 500$  or  $n = 1000$ , since the approximation in Theorem 3.2 does not work well, the local bootstrap version of test 1 is considered. Here 1000 samples of size  $n$  from (M2) are used, and for each sample, 1000 local bootstrap resamples are used to determine the rejection region. The level is 0.05. The power estimates for the test are given in Table 6.

In the above results, the power estimates for test 1 are larger when  $a$  is larger. This is expected. Under (M2) or (M3),  $E\rho_{p_n, q_n}^2(Z) = E\rho_{2,2}^2(Z)$  increases as  $a$  increases ( $a \in [0, 1]$ ), so test 1 should be more powerful for larger  $a$ , if the approximation in (3.22) and (3.30) work. Table 7 gives the values of  $E\rho_{p_n, q_n}^2(Z)$  for  $a = 0.1$  and  $0.3$ . For (M2), the calculation of  $E\rho_{p_n, q_n}^2(Z)$  is done for the transformed  $(X, Y, Z)$ , which is obtained by applying the function  $\Phi$  to the original  $(X, Y, Z)$ .

**6. Concluding remarks.** A test statistic for testing conditional independence based on maximal nonlinear conditional correlation is proposed. Two tests, tests 1 and 1N, are constructed using the test statistic. Both tests are consistent and have similar asymptotic properties, as discussed in Section 3.2. Some simulation experiments are carried out to check the performance of test 1. The simulation results show that when the sample size  $n = 10^4$ , the power of test 1 is comparable with that of test 2A. The simulation results also indicate that test 1 has better power when  $E\rho_{p_n, q_n}^2(Z)$  is larger, as expected.

Below are a few remarks.

TABLE 5  
Test 1 power estimates for  $n = 5000$  and  $n = 10^4$

	$a = 0$		$a = 0.1$		$a = 0.3$	
	(M2)	(M3)	(M2)	(M3)	(M2)	(M3)
$n = 5000$	0.052	0.039	0.373	0.321	0.998	1
$n = 10^4$	0.049	0.041	0.65	0.572	1	1

TABLE 6  
Power estimates for test 1 with local bootstrap

	$a = 0$	$a = 0.1$	$a = 0.3$
$n = 500$	0.041	0.071	0.309
$n = 1000$	0.033	0.099	0.531

1. Equation (3.20) requires that  $p_n$ ,  $q_n$  and  $n_Z$  grow slowly comparing to  $n$ . The parameter selection result in Table 2 in Section 5 seems to agree with such a requirement. With  $n = 10^4$ ,  $n_Z$  is only 5 and  $p_n = q_n = 2$ . When  $p_n = q_n = 3$ , even with  $h_{0,n} = 0.4$  (this corresponds to the smallest  $n_Z$  for  $n = 10^4$ ), the distribution of the test statistic cannot be approximated well by the distribution of  $\sum_{k=1}^{n_Z} \lambda_k$ .
2. The parameter selection criteria given in Section 5 needs to be studied to see whether the asymptotic properties of test 1 still hold using such a criteria.
3. When the distribution of the test statistic cannot be approximated well by the distribution of  $\sum_{k=1}^{n_Z} \lambda_k$ , it is possible to use local bootstrap version of test 1. However, it takes a lot of time to obtain the bootstrap resamples, so this approach is recommended when the sample size  $n$  is small.
4. In all theorems proved in this paper, it is assumed that the  $(X_i, Y_i, Z_i)$ 's are i.i.d. It is also expected that test 1 works for some stationary weakly dependent data such as the vector ARMA processes, where the central limit theorem for the i.i.d. case still applies. However, to carry out the details in the proofs, one needs the strong approximation result in Lemma 2, which is a stronger result than the central limit theorem and requires a version of Lemma 5 that works for dependent data.
5. Test 1 can be modified to work for discrete  $Z$ . Modification is necessary since the rate of convergence for each  $\hat{\rho}(z_k)$  is faster in the discrete case.
6. In Lemma 1 and Theorems 3.1 and 3.2, the  $z_k$ 's are chosen in  $\mathcal{Z}(\varepsilon_n)$  so that they are  $\varepsilon_n$ -away from the boundary, and it is assumed that  $h_n/\varepsilon_n = O(n^{-\beta})$  to ensure that certain error terms in the bias/variance calculation are negligible. For implementation, the condition  $h_n/\varepsilon_n = O(n^{-\beta})$  still leaves some room for choosing  $\varepsilon_n$ . This problem can be eliminated

TABLE 7  
 $E\rho_{p_n, q_n}^2(Z)$  under (M2) and (M3)

	$a = 0.1$	$a = 0.3$
(M2)	0.001345575	0.01908246
(M3)	0.002044604	0.01765322

by using a kernel function with compact support, as pointed out by a reviewer. In particular, if the kernel function  $k_0$  is supported on  $[-1, 1]^d$ , then one can simply take  $\varepsilon_n = h_n$ . In such case, even though the condition  $h_n/\varepsilon_n = O(n^{-\beta})$  does not hold, the results in Lemma 1 and Theorems 3.1 and 3.2 remain valid.

## 7. Proofs.

7.1. *Proof of Lemma 1.* Recall that for  $1 \leq j \leq k_n$ ,

$$W_{n,j}(z) = \sqrt{nh_n^d c_K f_Z(z)} \left( \left( \sum_{i=1}^n w_i(z) f_{n,j}(X_i, Y_i, z) \right) - E(f_{n,j}(X, Y, z) | Z = z) \right).$$

To prove the asymptotic normality of  $W_{n,j}(z_k)$ 's, we will approximate  $W_{n,j}(z)$  using sums of i.i.d. random variables. For  $1 \leq i \leq n$ , let  $w_{0,i}(z) = k_0(h_n^{-1}(z - Z_i))$  and let  $\hat{f}_Z(z) = n^{-1} h_n^{-d} \sum_{i=1}^n w_{0,i}(z)$ . Then  $w_i(z) = n^{-1} h_n^{-d} w_{0,i}(z) / \hat{f}_Z(z)$ . For  $1 \leq j \leq k_n$ , let

$$\begin{aligned} \tilde{W}_{n,j}(z) &= (nh_n^d f_Z(z))^{-1/2} (c_K)^{1/2} \sum_{i=1}^n (w_{0,i}(z) f_{n,j}(X_i, Y_i, z) \\ &\quad - E w_{0,i}(z) f_{n,j}(X_i, Y_i, z)) \end{aligned}$$

and  $\tilde{W}_{n,k_n+1}(z) = \sqrt{nh_n^d c_K} (f_Z(z))^{-1/2} (\hat{f}_Z(z) - E \hat{f}_Z(z))$ , then

$$\begin{aligned} W_{n,j}(z) &= \frac{f_Z(z)}{\hat{f}_Z(z)} \tilde{W}_{n,j}(z) + \sqrt{nh_n^d c_K f_Z(z)} E(f_{n,j}(X, Y, z) | Z = z) \left( \frac{f_Z(z)}{\hat{f}_Z(z)} - 1 \right) \\ &\quad + \frac{\sqrt{nh_n^d c_K f_Z(z)}}{\hat{f}_Z(z)} (h_n^{-d} E(w_{0,1}(z) f_{n,j}(X_1, Y_1, z)) \\ &\quad - E(f_{n,j}(X, Y, z) | Z = z) f_Z(z)) \\ &= \hat{W}_{n,j}(z) + \sum_{\ell=1}^4 R_{\ell,n,j}(z), \end{aligned}$$

where  $\hat{W}_{n,j}(z) = \tilde{W}_{n,j}(z) - \tilde{W}_{n,k_n+1}(z) E(f_{n,j}(X, Y, z) | Z = z)$ ,

$$R_{1,n,j}(z) = \left( \frac{f_Z(z)}{\hat{f}_Z(z)} - 1 \right) \tilde{W}_{n,j}(z),$$

$$\begin{aligned} R_{2,n,j}(z) &= \frac{\sqrt{nh_n^d c_K f_Z(z)}}{\hat{f}_Z(z)} (h_n^{-d} E(w_{0,1}(z) f_{n,j}(X_1, Y_1, z)) \\ &\quad - E(f_{n,j}(X, Y, z) | Z = z) f_Z(z)), \end{aligned}$$

$$R_{3,n,j}(z) = \frac{\sqrt{nh_n^d c_K} E(f_{n,j}(X, Y, z) | Z = z) (f_Z(z) - \hat{f}_Z(z))^2}{\hat{f}_Z(z) \sqrt{f_Z(z)}}$$

and

$$R_{4,n,j}(z) = -\frac{\sqrt{nh_n^d c_K}}{\sqrt{f_Z(z)}} E(f_{n,j}(X, Y, z)|Z = z)(Ef_Z(z) - f_Z(z)).$$

We will complete the proof by showing that the following results hold for  $T_n = \exp(-(\ln n)^{1/9})$ .

- (C1)  $\sum_{j=1}^{k_n} \sum_{k=1}^{n_Z} (\sum_{\ell=1}^4 R_{\ell,n,j}(z_k))^2 = O_p(T_n)$ .  
(C2) There exist random variables  $N_{1,j,k}$  and  $\varepsilon_{1,j,k} : 1 \leq j \leq k_n, 1 \leq k \leq n_Z$  such that the joint distribution of  $(N_{1,j,k} + \varepsilon_{1,j,k})_{j,k}$  is the same as that of  $(\hat{W}_{n,j}(z_k))_{j,k}$ ,  $N_{1,j,k}$ 's are jointly normal with  $EN_{1,j,k} = 0$  and  $\text{Cov}(N_{1,j,k}, N_{1,\ell,k^*}) = \text{Cov}(\hat{W}_{n,j}(z_k), \hat{W}_{n,\ell}(z_{k^*}))$  and  $\sum_{j=1}^{k_n} \sum_{k=1}^{n_Z} \varepsilon_{1,j,k}^2 = O_p(T_n)$ .  
(C3) There exist random variables  $N_{2,j,k}$  and  $\varepsilon_{2,j,k} : 1 \leq j \leq k_n, 1 \leq k \leq n_Z$  such that the joint distribution of  $(N_{2,j,k} + \varepsilon_{2,j,k})_{j,k}$  is the same as that of  $(N_{1,j,k})_{j,k}$ ,  $N_{2,j,k}$ 's are jointly normal with  $EN_{2,j,k} = 0$  and

$$\begin{aligned} & \text{Cov}(N_{2,j,k}, N_{2,\ell,k^*}) \\ &= \begin{cases} \text{Cov}(f_{n,j}(X, Y, z_k), f_{n,\ell}(X, Y, z_k)|Z = z_k), & \text{if } k = k^*; \\ 0, & \text{otherwise,} \end{cases} \end{aligned}$$

$$\text{and } \sum_{j=1}^{k_n} \sum_{k=1}^{n_Z} \varepsilon_{2,j,k}^2 = O_p(T_n).$$

Note that Lemma 1 follows from (C1)–(C3) since one can construct random variables  $\tilde{N}_{2,j,k}$ ,  $\tilde{\varepsilon}_{2,j,k}$ ,  $\tilde{\varepsilon}_{1,j,k}$  and  $R_{5,n,j,k} : 1 \leq j \leq k_n, 1 \leq k \leq n_Z$  on the same probability space such that the joint distribution of  $(\tilde{N}_{2,j,k}, \tilde{\varepsilon}_{2,j,k})_{j,k}$  is the same as that of  $(N_{2,j,k}, \varepsilon_{2,j,k})_{j,k}$ , the joint distribution of  $(\tilde{\varepsilon}_{1,j,k}, \tilde{N}_{2,j,k} + \tilde{\varepsilon}_{2,j,k})_{j,k}$  is the same as that of  $(\varepsilon_{1,j,k}, N_{1,j,k})_{j,k}$ , and the joint distribution of  $(R_{5,n,j,k}, \tilde{N}_{2,j,k} + \tilde{\varepsilon}_{2,j,k} + \tilde{\varepsilon}_{1,j,k})_{j,k}$  is the same as that of  $(\sum_{\ell=1}^4 R_{\ell,n,j}(z_k), \hat{W}_{n,j}(z_k))_{j,k}$ . Take  $W_{n,1,j,k} = \tilde{N}_{2,j,k}$  and  $W_{n,2,j,k} = \tilde{\varepsilon}_{2,j,k} + \tilde{\varepsilon}_{1,j,k} + R_{5,n,j,k}$ , then we have Lemma 1.

To establish (C1)–(C3), we need certain expectations and covariances, which are computed below. Under (R1)–(R3) and the conditions that  $\int uk_0(u) du = 0$  and  $\sigma_0^2 = \int \|u\|^2 k_0(u) du < \infty$ , for  $z \in \mathcal{Z}(\varepsilon_n)$ , we have

$$\begin{aligned} (7.1) \quad & (h_n^d)^{-1} E(w_{0,1}(z) f_{n,j}(X_1, Y_1, z)) \\ &= E(f_{n,j}(X, Y, z)|Z = z) f_Z(z) + r_{n,j,1}(z) C_n h_n^2, \end{aligned}$$

where

$$\begin{aligned} r_{n,j,1}(z) &= c_0 \int h(x, y) d\mu(x, y) \\ &\quad \times (2d\sigma_0^2 \theta_{n,j,1} + \theta_{n,j,2} h_n^{-2} (2 + h_n) \gamma_4^d \exp(-\gamma_5 \varepsilon_n^2 h_n^{-2})), \end{aligned}$$

$|\theta_{n,j,1}|, |\theta_{n,j,2}| \leq 1$ , and  $\gamma_4$  and  $\gamma_5$  are positive constants that depend on  $\gamma_2$  and  $\gamma_3$  only. Also, for  $k \neq k^*$ ,  $z_k, z_{k^*} \in \mathcal{Z}(\varepsilon_n)$ , we have

$$\begin{aligned}
(7.2) \quad & (h_n^d)^{-2} \text{Cov}(w_{0,1}(z_k) f_{n,j}(X_1, Y_1, z_k), w_{0,1}(z_{k^*}) f_{n,\ell}(X_1, Y_1, z_{k^*})) \\
&= \theta_{j,\ell,k,k^*} (h_n^d)^{-2} (\gamma_2)^{2d} \exp(-0.5\gamma_3 h_n^{-2} \|z_k - z_{k^*}\|^2) C_n^2 \\
&\quad - f_Z(z_k) f_Z(z_{k^*}) E(f_{n,j}(X, Y, z_k) | Z = z_k) E(f_{n,\ell}(X, Y, z_{k^*}) | Z = z_{k^*}) \\
&\quad - f_Z(z_k) E(f_{n,j}(X, Y, z_k) | Z = z_k) r_{n,\ell,1}(z_{k^*}) C_n h_n^2 \\
&\quad - f_Z(z_{k^*}) E(f_{n,\ell}(X, Y, z_{k^*}) | Z = z_{k^*}) r_{n,j,1}(z_k) C_n h_n^2 \\
&\quad - r_{n,j,1}(z_k) r_{n,\ell,1}(z_{k^*}) C_n^2 h_n^4,
\end{aligned}$$

where  $|\theta_{j,\ell,k,k^*}| \leq 1$ . Finally, for  $z \in \mathcal{Z}(\varepsilon_n)$ ,

$$\begin{aligned}
(7.3) \quad & (h_n^d)^{-1} \text{Cov}(w_{0,1}(z) f_{n,j}(X_1, Y_1, z), w_{0,1}(z) f_{n,\ell}(X_1, Y_1, z)) \\
&= f_Z(z) E(f_{n,j}(X, Y, z) f_{n,\ell}(X, Y, z) | Z = z) \int k_0^2(u) du + r_{n,j,\ell,2}(z) C_n^2 h_n \\
&\quad - h_n^d f_Z^2(z) E(f_{n,j}(X, Y, z) | Z = z) E(f_{n,\ell}(X, Y, z) | Z = z) \\
&\quad - h_n^{d+2} C_n r_{n,j,1}(z) f_Z(z) E(f_{n,\ell}(X, Y, z) | Z = z) \\
&\quad - h_n^{d+2} C_n r_{n,\ell,1}(z) f_Z(z) E(f_{n,j}(X, Y, z) | Z = z) \\
&\quad - h_n^{d+4} C_n^2 r_{n,j,1}(z) r_{n,\ell,1}(z)
\end{aligned}$$

and

$$(7.4) \quad h_n^{-d} E(w_{0,1}(z) f_{n,j}(X_1, Y_1, z))^3 \leq C_n^3 c_0 \int k_0^3(u) du,$$

where

$$|r_{n,j,\ell,2}(z)| \leq 2c_0 \int h(x, y) d\mu(x, y) \left( \sqrt{d} \int \|u\| k_0^2(u) du + h_n^{-1} \gamma_6^d e^{-\gamma_7 \varepsilon_n^2 / h_n^2} \right)$$

for some positive constants  $\gamma_6$  and  $\gamma_7$  that depend on  $\gamma_2$  and  $\gamma_3$  only. Below we will prove (C1)–(C3).

PROOF OF (C1). Let  $S_n = \sum_{k=1}^{n_Z} (\hat{f}_Z(z_k) - f_Z(z_k))^2$  and  $A_n = \{\sqrt{S_n} < \min\{1, (2c_1)^{-1}\}\}$ . From (7.1) and (7.3),  $ES_n = O(n_Z(h_n^4 + (nh_n^d)^{-1})) = O(n_Z(n \times h_n^d)^{-1})$  and  $1/f_Z(z_k) \leq c_1$  for all  $k$ ,  $P(A_n^c) \rightarrow 0$  as  $n \rightarrow \infty$ . From (7.1), on  $A_n$ ,

$$\sum_{j=1}^{k_n} \sum_{k=1}^{n_Z} \left( \sum_{\ell=1}^4 |R_{\ell,n,j}(z_k)| \right)^2$$

$$\leq O(1) \left( S_n \left( \sum_{j=1}^{k_n} \sum_{k=1}^{n_Z} \tilde{W}_{n,j}^2(z_k) \right) + k_n n_Z C_n^2 (n h_n^{d+4}) + k_n C_n^2 n h_n^d S_n^2 \right),$$

and it follows from (7.3) that

$$E \left( \sum_{j=1}^{k_n} \sum_{k=1}^{n_Z} \tilde{W}_{n,j}^2(z_k) \right) = O(k_n n_Z C_n^2).$$

Take

$$T_{1,n} = \frac{k_n n_Z^2 C_n^2}{n h_n^d} + k_n n_Z C_n^2 n h_n^{d+4},$$

then (C1) holds with  $T_n = \exp(-(\ln n)^{1/9})$  since  $T_{1,n} = O(T_n)$ .  $\square$

The proof of (C2) is based on the following lemma, which deals with the normal approximation of sum of i.i.d. random vectors.

LEMMA 2. *Suppose that  $X_1, \dots, X_n$  are i.i.d. random vectors in  $R^{d_1}$  with mean 0 and variance  $\Sigma$ . Suppose that there exist positive constants  $C$ ,  $a_2$  and  $a_3$  such that  $1 \leq a_2 \leq a_3 \leq C$ ,  $\|X_1\| \leq C$  and  $E\|X_1\|^k \leq a_k^k$  for  $k = 2, 3$ . Then for  $T \geq 1$ , there exist random vectors  $S$  and  $Y$  on the same probability space such that  $S$  is distributed as  $(X_1 + \dots + X_n)/\sqrt{n}$ ,  $Y$  is multivariate normal with mean 0 and variance  $\Sigma$  and for  $n \geq (25/(16a_2^2) + 25d_1/12)C^2T^4 \exp(3T^2/16)$ ,*

$$P(\|S - Y\| \geq \alpha) \leq \alpha,$$

if

$$\alpha \geq \frac{33.75a_3^3}{\sqrt{n}} (12)^{d_1} e^{(d_1+3)T^2/8} + (48)^{d_1} e^{-3T^2/(32a_2^2)}.$$

The proof of Lemma 2 is given in Section 7.1.1. To prove (C2), note that  $\tilde{W}_{n,j}(z_k) = \sum_{i=1}^n (g_{n,j,k}(X_i, Y_i, Z_i) - E g_{n,j,k}(X_i, Y_i, Z_i))/\sqrt{n}$ , where

$$\begin{aligned} g_{n,j,k}(X_i, Y_i, Z_i) &= \frac{\sqrt{c_K}}{\sqrt{f_Z(z_k) h_n^d}} k_0 \left( \frac{z_k - Z_i}{h_n} \right) \\ &\quad \times (f_{n,j}(X_i, Y_i, z_k) - E(f_{n,j}(X, Y, z_k) | Z = z_k)). \end{aligned}$$



From (7.1)–(7.4), we have

$$\begin{aligned} \left( \sum_{j=1}^{k_n} \sum_{k=1}^{n_Z} (g_{n,j,k}(X_i, Y_i, Z_i) - E g_{n,j,k}(X_i, Y_i, Z_i))^2 \right)^{1/2} &\leq \frac{O(1)C_n \sqrt{k_n n_Z}}{\sqrt{h_n^d}}, \\ \left( \sum_{j=1}^{k_n} \sum_{k=1}^{n_Z} E(g_{n,j,k}(X_i, Y_i, Z_i) - E g_{n,j,k}(X_i, Y_i, Z_i))^2 \right)^{1/2} &\leq O(1)C_n \sqrt{k_n n_Z} \end{aligned}$$

and

$$\begin{aligned} &\left( E \left( \sum_{j=1}^{k_n} \sum_{k=1}^{n_Z} (g_{n,j,k}(X_i, Y_i, Z_i) - E g_{n,j,k}(X_i, Y_i, Z_i))^2 \right)^{3/2} \right)^{1/3} \\ &\leq C_n \sqrt{k_n n_Z} h_n^{-d/6} O(1). \end{aligned}$$

Note that for every constant  $M > 0$ , the condition

$$n \geq \left( \frac{25}{16} + \frac{25k_n n_Z}{12} \right) \left( \frac{MC_n \sqrt{k_n n_Z}}{\sqrt{h_n^d}} \right)^2 T_{3,n}^4 e^{3T_{3,n}^2/16}$$

holds for large  $n$  with  $T_{3,n} = (\ln n)^{1/8}$ , so Lemma 2 is applicable. From Lemma 2, (C2) holds with any  $T_n$  such that  $T_{2,n} = O(T_n)$ , where

$$T_{2,n} = \frac{(C_n \sqrt{k_n n_Z})^6 12^{2k_n n_Z} e^{(k_n n_Z + 3)T_{3,n}^2/4}}{n h_n^d} + (48)^{2k_n n_Z} e^{-\gamma T_{3,n}^2 / (C_n \sqrt{k_n n_Z})^2},$$

$\gamma > 0$  is a constant. Since  $T_{2,n} = O(\exp(-\gamma_1 (\ln n)^{1/8}))$  for some constant  $\gamma_1 > 0$ , (C2) holds with  $T_n = \exp(-(\ln n)^{1/9})$ .

The proof of (C3) is based on the following result.

**FACT 3.** *Suppose that  $A$  and  $B$  are  $d_1 \times d_1$  nonnegative definite matrices. Then*

$$\|\sqrt{A} - \sqrt{B}\| \leq d_1^{3/4} \sqrt{\|A - B\|}.$$

The proof of Fact 3 is given at the end of the proof of (C3). Note that Fact 3 implies the following: suppose that  $X_0$  and  $Y_0$  are two  $d_1 \times 1$  normal vectors of mean 0 and covariance matrices  $A$  and  $B$ , respectively. Let  $Z$  be a  $d_1 \times 1$  normal vector whose elements are i.i.d.  $N(0, 1)$ . Then  $\sqrt{A}Z$  is distributed as  $X_0$  and  $\sqrt{B}Z$  is distributed as  $Y_0$  and

$$\begin{aligned} \|\sqrt{A}Z - \sqrt{B}Z\|^2 &\leq \|\sqrt{A} - \sqrt{B}\|^2 \|Z\|^2 \leq d_1^{3/2} \|A - B\| \|Z\|^2 \\ &= O_p(d_1^{5/2} \|A - B\|). \end{aligned}$$

Therefore, (C3) holds if  $\text{Cov}(\hat{W}_{n,j}(z_k), \hat{W}_{n,\ell}(z_{k^*}))$  is close to

$$\text{Cov}(f_{n,j}(X, Y, z_k), f_{n,\ell}(X, Y, z_k) | Z = z_k) \delta_{k,k^*},$$

where  $\delta_{k,k^*}$  is 1 if  $k = k^*$  and is 0 otherwise. From (7.1)–(7.4), we have

$$\begin{aligned} & \sum_{j,\ell,k,k^*} (\text{Cov}(\hat{W}_{n,j}(z_k), \hat{W}_{n,\ell}(z_{k^*})) \\ & \quad - \text{Cov}(f_{n,j}(X, Y, z_k), f_{n,\ell}(X, Y, z_k) | Z = z_k) \delta_{k,k^*})^2 \\ & = h_n C_n^2 (k_n n_Z)^2 O(1), \end{aligned}$$

so (C3) holds with  $T_n = \exp(-(\ln n)^{1/9})$  since  $(k_n n_Z)^{5/2} \sqrt{h_n C_n^2 (k_n n_Z)^2} = O(\exp(-(\ln n)^{1/9}))$ .

**PROOF OF FACT 3.** Consider first the case where  $A$  is diagonal. Let  $D$  be a diagonal matrix such that  $B = Q^T D Q$  for some  $Q$  such that  $Q Q^T = I$ . Let  $D = \text{diag}(\lambda_1, \dots, \lambda_{d_1})$ ,  $A = \text{diag}(\alpha_1, \dots, \alpha_{d_1})$ ,  $Q = (q_{i,j})$  and  $E = B - A = (e_{i,j})$ . Let  $q_i$  be the  $i$ th column of  $Q$ , then  $q_i^T D q_j = \alpha_i \delta_{i,j} + e_{i,j}$ , where  $\delta_{i,j} = 1$  for  $i = j$  and  $\delta_{i,j} = 0$ , otherwise. Write  $D q_k = \sum_{j=1}^{d_1} (q_k^T D q_j) q_j$ , then

$$\begin{aligned} \|\sqrt{D} q_k - \sqrt{\alpha_k} q_k\|^2 &= \sum_{j=1}^{d_1} (\sqrt{\lambda_j} q_{j,k} - \sqrt{\alpha_k} q_{j,k})^2 \\ &= \sum_{j=1}^{d_1} (\sqrt{\lambda_j} |q_{j,k}| - \sqrt{\alpha_k} |q_{j,k}|)^2 |q_{j,k}| \\ &\leq \sum_{j=1}^{d_1} |\lambda_j |q_{j,k}| - \alpha_k |q_{j,k}|| |q_{j,k}| \\ &\leq \left( \sum_{j=1}^{d_1} (\lambda_j |q_{j,k}| - \alpha_k |q_{j,k}|)^2 \right)^{1/2} \left( \sum_{j=1}^{d_1} |q_{j,k}|^2 \right)^{1/2} \\ &= \left( \sum_{j=1}^{d_1} e_{k,j}^2 \right)^{1/2} \end{aligned}$$

and

$$\begin{aligned} \|\sqrt{Q^T D Q} - \sqrt{A}\|^2 &= \sum_{i=1}^{d_1} \sum_{j=1}^{d_1} (q_i^T \sqrt{D} q_j - q_i^T \sqrt{\alpha_j} q_j)^2 \\ &\leq \sum_{i=1}^{d_1} \sum_{j=1}^{d_1} \|\sqrt{D} q_j - \sqrt{\alpha_j} q_j\|^2 \end{aligned}$$

$$\begin{aligned}
&\leq d_1 \sum_{j=1}^{d_1} \left( \sum_{\ell=1}^{d_1} e_{j,\ell}^2 \right)^{1/2} \\
&\leq (d_1)^{3/2} \left( \sum_{j=1}^{d_1} \sum_{\ell=1}^{d_1} e_{j,\ell}^2 \right)^{1/2},
\end{aligned}$$

so the result in Fact 3 holds if  $A$  (or  $B$ ) is diagonal. For general  $A$  and  $B$ , write  $A = P^T A_0 P$  and  $B = Q^T D Q$ , where  $A_0$  and  $D$  are diagonal and  $P^T P = Q^T Q = I$ . Let  $B_0 = P Q^T D Q P^T$ , then we have

$$\begin{aligned}
\|\sqrt{A} - \sqrt{B}\| &= \|P^T \sqrt{A_0} P - Q^T \sqrt{D} Q\| \\
&= \|\sqrt{A_0} - P Q^T \sqrt{D} Q P^T\| \leq d_1^{3/4} \sqrt{\|A_0 - B_0\|} \\
&= d_1^{3/4} \sqrt{\|P^T A_0 P - P^T B_0 P\|} = d_1^{3/4} \sqrt{\|A - B\|}.
\end{aligned}$$

The proofs of Fact 3 and Lemma 1 are complete.  $\square$

7.1.1. *Proof of Lemma 2.* The proof Lemma 2 is based on several facts, which are taken directly or adapted from some existing results and are stated/proved below in Lemmas 3–5.

In the statements of Lemmas 3 and 4,  $(S_0, d_0)$  is a metric space,  $\mathcal{B}$  denotes the collection of Borel sets in  $(S_0, d_0)$ , and for two measures  $\mu_1$  and  $\mu_2$  defined on  $\mathcal{B}$ ,  $\rho_0(\mu_1, \mu_2)$  denotes the Prohorov distance of  $\mu_1$  and  $\mu_2$ , which is defined as

$$\rho_0(\mu_1, \mu_2) = \inf\{\epsilon > 0 : \mu_1(A) < \mu_2(A^\epsilon) + \epsilon, \text{ for all } A \in \mathcal{B}\},$$

where  $A^\epsilon = \{x : d^*(x, A) < \epsilon\}$  and  $d^*(x, A) = \inf\{d_0(x, y) : y \in A\}$ . Here are Lemmas 3–5.

LEMMA 3 (Lemma 2.1 in Berkes and Philipp [1]). *Suppose that  $P_1$  and  $P_2$  are two measures defined on  $\mathcal{B}$  and  $\rho_0(P_1, P_2) < \alpha$ . Then there exists a probability measure  $Q$  on the Borel sets of  $S_0 \times S_0$  with marginals  $P_1$  and  $P_2$  such that*

$$Q\{(x, y) : d_0(x, y) > \alpha\} \leq \alpha.$$

LEMMA 4 (Adapted from Lemma 2.2 in [1]). *Suppose that  $F$  and  $G$  are two distributions on  $R^{d_1}$  with characteristic functions  $f$  and  $g$ , respectively. Then for  $\sigma \in (0, 1]$  and  $T > 0$ , the Prohorov distance  $\rho_0(F, G) \leq \alpha$ , where*

$$\begin{aligned}
\alpha &= \sigma T + 3(2^{d_1})e^{-3T^2/32} + \left(\frac{T}{\pi}\right)^{d_1} \int |f(u) - g(u)| e^{-\sigma^2 \|u\|^2/2} du \\
&\quad + F\left(\left\{x : \|x\| \geq \frac{T}{2}\right\}\right).
\end{aligned}$$

PROOF. Let  $H$  be the  $N(0, \sigma^2 I)$  distribution on  $R^{d_1}$ , where  $I$  is the identity matrix and  $\sigma > 0$ . Let  $F_1$  be the convolution of  $F$  and  $H$  and  $G_1$  be the convolution of  $G$  and  $H$ . Then

$$(7.5) \quad \rho_0(F, G) \leq \rho_0(F_1, G_1) + 2 \max\{r, H(\{x : \|x\| \geq r\})\} \quad \text{for every } r > 0.$$

Let  $f_1, g_1$  and  $h$  be the characteristic functions of  $F_1, G_1$  and  $H$ , respectively, and let  $\gamma_F$  and  $\gamma_G$  be the densities of  $F_1$  and  $G_1$ , respectively. Then

$$\begin{aligned} |\gamma_F(x) - \gamma_G(x)| &= (2\pi)^{-d_1} \left| \int e^{-iu^T x} (f_1(u) - g_1(u)) du \right| \\ &\leq (2\pi)^{-d_1} \int |f(u) - g(u)| |h(u)| du, \end{aligned}$$

which implies that for every borel set  $B$  in  $R^{d_1}$ ,

$$\begin{aligned} F_1(B) - G_1(B) &\leq F_1(B \cap \{x : \|x\| \leq T\}) - G_1(B \cap \{x : \|x\| \leq T\}) + F_1(\{x : \|x\| \geq T\}) \\ &\leq \int_{\{x : \|x\| \leq T\}} |\gamma_F(x) - \gamma_G(x)| dx + F(\{x : \|x\| \geq T/2\}) \\ &\quad + H(\{x : \|x\| \geq T/2\}) \\ &\leq \underbrace{\left( \frac{T}{\pi} \right)^{d_1} \int |f(u) - g(u)| |h(u)| du + F(\{x : \|x\| \geq T/2\}) + H(\{x : \|x\| \geq T/2\})}_{II}. \end{aligned}$$

Note that  $II$  is an upper bound for the Prohorov distance  $\rho_0(F_1, G_1)$ , so for  $r \leq T/2$ , it follows from (7.5) that

$$\begin{aligned} \rho_0(F, G) &\leq II + 2r + 2H(\{x : \|x\| \geq r\}) \\ &\leq \left( \frac{T}{\pi} \right)^{d_1} \int |f(u) - g(u)| |h(u)| du + F(\{x : \|x\| \geq T/2\}) + 2r \\ &\quad + 3P(\chi^2(d_1) \geq (r/\sigma)^2). \end{aligned}$$

Since  $h(u) = e^{-\sigma^2 \|u\|^2/2}$  and

$$\begin{aligned} (7.6) \quad P(\chi^2(d_1) \geq A) &\leq e^{-tA} E e^{t\chi^2(d_1)}|_{t=3/8} \\ &= e^{-3A/8} (2^{d_1}) \quad \text{for every } A > 0. \end{aligned}$$

Lemma 4 holds if  $r = \sigma T/2$  and  $\sigma \in (0, 1]$ .  $\square$

LEMMA 5 (Adapted from Theorem 1(a) in pages 204–208 in Gnedenko and Kolmogorov [5]). *Suppose that  $X_1, \dots, X_n$  are i.i.d. random vectors*

with mean 0 and variance  $\Sigma$ . Suppose that  $C$  and  $a$  are positive constants such that  $\|X_1\| \leq C$ ,  $a \leq C$  and  $E\|X_1\|^k \leq a^k$  for  $k = 2, 3$ . Let  $f_n$  be the characteristic function of  $(X_1 + \dots + X_n)/\sqrt{n}$ . Then

$$\left| f_n(u) - \exp\left(-\frac{1}{2}u^T \Sigma u\right) \right| \leq \frac{0.25\|u\|^3 a^3}{\sqrt{n}},$$

if  $\|u\| \leq (0.4\sqrt{n})/C$ .

PROOF. Consider first the case where  $X_1$  is univariate. Let  $U = f_1(u/\sqrt{n}) - 1$ , then

$$U = \frac{\theta_1^* E X_1^2}{2} \left( \frac{u}{\sqrt{n}} \right)^2$$

and

$$U = \frac{E X_1^2}{2} \left( \frac{iu}{\sqrt{n}} \right)^2 + \frac{\theta_1 E |X_1|^3}{3!} \left( \frac{u}{\sqrt{n}} \right)^3,$$

where  $|\theta_1^*| \leq 1$  and  $|\theta_1| \leq 1$ . Suppose that  $|u| \leq (0.4\sqrt{n})/C$ , then  $|U| < 0.1$  and

$$\log(1 + U) = U + 0.62\theta_2 U^2,$$

where  $|\theta_2| \leq 1$ . Let  $V = \log f_n(u) + E(X_1^2)u^2/2 = E(X_1^2)u^2/2 + n \log(1 + U)$ , then

$$\begin{aligned} V &= \frac{n\theta_1 E |X_1|^3 u^3}{3!n^{3/2}} + (0.62)n\theta_2 \left( \frac{E X_1^2}{2} \left( \frac{iu}{\sqrt{n}} \right)^2 + \frac{\theta_1 E |X_1|^3}{3!} \left( \frac{u}{\sqrt{n}} \right)^3 \right)^2 \\ &= \frac{\lambda_1 |u|^3 a^3}{6\sqrt{n}} + 0.62 \left( \frac{\lambda_2 a^4 u^4}{4n} + \frac{\lambda_3 a^5 |u|^5}{6(\sqrt{n})^3} + \frac{\lambda_4 a^6 u^6}{36n^2} \right) \\ &= \frac{|u|^3 a^3}{\sqrt{n}} \left( \frac{\lambda_1}{6} + 0.62 \left( \frac{\lambda_2 a |u|}{4\sqrt{n}} + \frac{\lambda_3 a^2 u^2}{6n} + \frac{\lambda_4 a^3 |u|^3}{36(\sqrt{n})^3} \right) \right), \end{aligned}$$

where  $|\lambda_k| \leq 1$  for  $k = 1, 2, 3, 4$ . Since  $a|u|/\sqrt{n} \leq 0.4$ ,

$$V = \frac{\theta_3 (0.25)|u|^3 a^3}{\sqrt{n}},$$

where  $|\theta_3| \leq 1$ . Since  $e^V = 1 + \theta_4 |V| e^{|V|}$ , where  $|\theta_4| \leq 1$ ,

$$\begin{aligned} f_n(u) &= \exp\left(-\frac{E(X_1^2)u^2}{2}\right) (1 + \theta_4 |V| e^{|V|}) \\ &= \exp\left(-\frac{E(X_1^2)u^2}{2}\right) + \theta_5 \left( \frac{0.25|u|^3 a^3}{\sqrt{n}} \right) e^{|V| - E(X_1^2)u^2/2}, \end{aligned}$$

where  $|\theta_5| \leq 1$ . To find an upper bound for  $|V| - E(X_1^2)u^2/2$ , note that

$$\left| nU + \frac{E(X_1^2)u^2}{2} \right| = \frac{|\theta_1|E|X_1|^3|u|^3}{6\sqrt{n}} \leq \frac{CEX_1^2|u|^3}{6\sqrt{n}} \leq \frac{(0.4)u^2E(X_1^2)}{6},$$

$n|U| = |\theta_1^*|u^2E(X_1^2)/2 \leq u^2E(X_1^2)/2$  and

$$|n(\log(1+U) - U)| = 0.62n|\theta_2U^2| \leq 0.62(0.1) \left( \frac{E(X_1^2)u^2}{2} \right)$$

since  $|U| < 0.1$ . Therefore,

$$\begin{aligned} |V| - \frac{u^2E(X_1^2)}{2} &= \left| \frac{E(X_1^2)u^2}{2} + nU + n(\log(1+U) - U) \right| - \frac{u^2E(X_1^2)}{2} \\ &\leq \frac{(0.4)u^2E(X_1^2)}{6} + \frac{0.062E(X_1^2)u^2}{2} - \frac{u^2E(X_1^2)}{2} \leq 0 \end{aligned}$$

and Lemma 5 holds for the univariate case. The result for the general case can be obtained by applying the univariate result with  $u$  and  $X_i$  replaced by  $\|u\|$  and  $Y_i = u^T X_i / \|u\|$ .  $\square$

Now we are ready to prove Lemma 2.

PROOF OF LEMMA 2. Let  $f_n$  be the characteristic function of  $(X_1 + \dots + X_n)/\sqrt{n}$  and  $g$  be the characteristic function of  $G$ , the  $N(0, \Sigma)$  distribution. From Lemmas 3–5, there exist random vectors  $S$  and  $Y$  on the same probability space such that  $S$  is distributed as  $(X_1 + \dots + X_n)/\sqrt{n}$ ,  $Y$  is multivariate normal with mean 0 and variance  $\Sigma$  and

$$P(\|S - Y\| \geq \alpha_1) \leq \alpha_1,$$

where

$$\begin{aligned} \alpha_1 &= \sigma T + 3(2^{d_1})e^{-3T^2/32} + \frac{0.25a_3^3}{\sqrt{n}} \left( \frac{2}{\pi} \right)^{d_1/2} \frac{T^{d_1}}{\sigma^{d_1+3}} E(\chi^2(d_1))^{3/2} \\ &\quad + 2 \left( \frac{2}{\pi} \right)^{d_1/2} \frac{T^{d_1}}{\sigma^{d_1}} P \left( \chi^2(d_1) \geq \frac{0.16n\sigma^2}{C^2} \right) + P(\|N(0, \Sigma)\| \geq T/2). \end{aligned}$$

From the facts that  $E(\chi^2(d_1))^{3/2} \leq (E(\chi^2(d_1))^2)^{3/4}$  and  $P(\|N(0, \Sigma)\| \geq T/2) \leq P(\chi^2(d_1) \geq T^2/(4a_2^2))$ , (7.6) and the condition  $a_2 \geq 1$ , we have

$$\begin{aligned} \alpha_1 &\leq \sigma T + 4(2^{d_1})e^{-3T^2/(32a_2^2)} + \frac{0.25a_3^3}{\sqrt{n}} \left( \frac{2}{\pi} \right)^{d_1/2} \frac{T^{d_1}}{\sigma^{d_1+3}} (2d_1 + d_1^2)^{3/4} \\ &\quad + 2 \left( \frac{2}{\pi} \right)^{d_1/2} \frac{T^{d_1}}{\sigma^{d_1}} (2^{d_1})e^{-0.06n\sigma^2/(C^2)}. \end{aligned}$$

Set  $\sigma = T^{-1}e^{-3T^2/32}$ , then  $0 < \sigma \leq 1$ ,  $T/\sigma < 12e^{T^2/8}$  and  $1/\sigma < 3e^{T^2/8}$ , which, together with the fact that  $(2/\pi)^{d_1/2}(2d_1 + d_1^2)^{3/4} < 5$ , gives that

$$\begin{aligned} \alpha_1 &\leq (1 + 4(2^{d_1}))e^{-3T^2/(32a_2^2)} + \frac{33.75a_3^3}{\sqrt{n}}(12)^{d_1}e^{(d_1+3)T^2/8} \\ &\quad + 2(19.15)^{d_1}e^{d_1T^2/8}e^{-0.06n\sigma^2/(C^2)} \\ &\leq \frac{33.75a_3^3}{\sqrt{n}}(12)^{d_1}e^{(d_1+3)T^2/8} + (48)^{d_1}e^{-3T^2/(32a_2^2)} \leq \alpha, \end{aligned}$$

if  $0.06n\sigma^2/(C^2) \geq d_1T^2/8 + 3T^2/(32a_2^2)$ , which corresponds to  $n \geq (25/(16 \times a_2^2) + 25d_1/12)C^2T^4 \exp(3T^2/16)$  and we have Lemma 2.  $\square$

**7.2. Proof of Theorem 3.1.** To prove Theorem 3.1, we apply Lemma 1 by taking the  $f_{n,j}(X, Y, z)$ 's to be the functions  $\phi_\ell^*(X)\phi_{\ell'}^*(X)$ ,  $\phi_\ell^*(X)\psi_m^*(Y)$  and  $\psi_m^*(Y)\psi_{m'}^*(Y)$ , where  $1 \leq \ell \leq \ell' \leq p_n$  and  $1 \leq m \leq m' \leq q_n$ . In such case, (3.19) holds under conditions (B1) and (B2). To see this, for each  $1 \leq k \leq n_Z$  and  $1 \leq j \leq p_n$ , let  $\phi_{n,j,k}^*$  be the  $j$ th component of  $\phi^*$  when  $z = z_k$ . Then  $\phi_{n,j,k}^*(x) = \sum_{i=1}^{p_n} a_{n,i,j,k} \phi_{n,i}(x)$  for some  $a_{n,i,j,k}$ 's and

$$\begin{aligned} 1 &= E((\phi_{n,j,k}^*(X))^2 | Z = z_k) \\ &= E\left(\left(\sum_{i=1}^{p_n} a_{n,i,j,k} \phi_{n,i}(X)\right)^2 \middle| Z = z_k\right) \\ &\geq \delta_n \sum_{i=1}^{p_n} a_{n,i,j,k}^2, \end{aligned}$$

so  $|\phi_{n,j,k}^*(x)| \leq \sqrt{\sum_{i=1}^{p_n} a_{n,i,j,k}^2} \sqrt{\sum_{i=1}^{p_n} \phi_{n,i}^2(x)} \leq \sqrt{p_n/\delta_n}$ . Similarly, for each  $1 \leq k \leq n_Z$  and  $1 \leq j \leq q_n$ , let  $\psi_{n,j,k}^*$  be the  $j$ th component of  $\psi^*$  when  $z = z_k$ , then  $|\psi_{n,j,k}^*(x)| \leq \sqrt{q_n/\delta_n}$ . Thus, (3.19) holds with  $C_n = \max\{1, (p_n + q_n)/\delta_n\}$  and it follows from Lemma 1 that  $\sum_{k=1}^{n_Z} \|\hat{V}^*(z_k) - V^*(z_k)\|^2$  has the same distribution as  $\sum_{k=1}^{n_Z} (nh_n^d c_K f_Z(z_k))^{-1} \|W_{n,1,k} + W_{n,2,k}\|^2$ , where the  $W_{n,1,k}$ 's and  $W_{n,2,k}$ 's are random matrices such that each element in  $W_{n,1,k}$  is normal with mean zero and variance bounded by  $C_n^2 = (\max\{1, (p_n + q_n)/\delta_n\})^2$ , and  $\sum_{k=1}^{n_Z} \|W_{n,2,k}\|^2 = O_P(\exp(-(\ln n)^{1/9}))$ . Therefore,

$$(7.7) \quad \sum_{k=1}^{n_Z} \|\hat{V}^*(z_k) - V^*(z_k)\|^2 = O_P((nh_n^d)^{-1}(\ln n)^{1/8}).$$

To control the difference between  $g(\hat{V}^*(z_k), \alpha^*)$  and  $g(V^*(z_k), \alpha^*)$  for  $1 \leq k \leq n_Z$ , for a  $(p_n + q_n) \times (p_n + q_n)$  matrix  $U$ , let

$$(7.8) \quad g_{i,j}^*(U) = \begin{cases} g_{i,j}(U), & \text{if } (i, j) = (1, 2) \text{ or } (2, 1); \\ g_{i,j}^{-1}(U), & \text{if } (i, j) = (1, 1) \text{ or } (2, 2). \end{cases}$$

For  $1 \leq k \leq n_Z$ , let  $\Delta_{i,j,k} = g_{i,j}^*(\hat{V}^*(z_k)) - g_{i,j}^*(V^*(z_k))$  for  $1 \leq i, j \leq 2$ . Then from the fact that  $\|AB\| \leq \|A\|\|B\|$  for two matrices  $A$  and  $B$ , we have

$$\begin{aligned}
 & \|g(\hat{V}^*(z_k), \alpha^*) - g(V^*(z_k), \alpha^*)\| \\
 (7.9) \quad & \leq \prod_{i=1}^2 \prod_{j=1}^2 (\|g_{i,j}^*(V^*(z_k))\| + \|\Delta_{i,j,k}\|) - \prod_{i=1}^2 \prod_{j=1}^2 \|g_{i,j}^*(V^*(z_k))\| \\
 & \quad + \|g_{1,1}(\hat{V}^*(z_k)) - g_{1,1}(V^*(z_k))\| \|\alpha^*(\alpha^*)^T\|.
 \end{aligned}$$

To control the  $\Delta_{1,1,k}$  and  $\Delta_{2,2,k}$  in (7.9), the following result is needed.

**FACT 4.** *Suppose that  $A$  is a  $p \times p$  invertible matrix and  $\Delta = A - I_p$ . Then  $\|A^{-1} - I_p + \Delta\| \leq \|A^{-1} - I_p\| \|\Delta\|$  and*

$$\|A^{-1} - I_p\| \leq \frac{\|\Delta\|}{1 - \|\Delta\|} \quad \text{if } \|\Delta\| < 1.$$

**PROOF.** Let  $B = A^{-1} - I_p$ . Then  $B = -\Delta - B\Delta$ , so  $\|B + \Delta\| = \|B\Delta\| \leq \|B\| \|\Delta\|$ . Also,

$$(7.10) \quad \|B\| \leq \|\Delta\| (1 + \|B\|).$$

Apply (7.10) and we have

$$\|B\| \leq \frac{\|\Delta\|}{1 - \|\Delta\|} \quad \text{if } \|\Delta\| < 1.$$

Since  $\|\alpha^*\| = 1$  and for  $1 \leq k \leq n_Z$ ,  $g_{1,1}(V^*(z_k)) = I_{p_n}$ ,  $g_{2,2}(V^*(z_k)) = I_{q_n}$  and  $\|g_{1,2}(V^*(z_k))\|^2 = \|g_{2,1}(V^*(z_k))\|^2 \leq (p_n + q_n)$ , from (7.9) and Fact 4, we have

$$\begin{aligned}
 & \sum_{k=1}^{n_Z} \|g(\hat{V}^*(z_k), \alpha^*) - g(V^*(z_k), \alpha^*)\|^2 \\
 & = O_P((nh_n^d)^{-1} (\ln n)^{1/8} n_Z^2 (p_n + q_n)^3) \\
 & = O_P((nh_n^d)^{-1} (\ln n)^{1/4}),
 \end{aligned}$$

which gives (3.21) since  $|\hat{\rho}^2(z_k) - \rho_{p_n, q_n}^2(z_k)| \leq \|g(\hat{V}^*(z_k), \alpha^*) - g(V^*(z_k), \alpha^*)\|$  for  $1 \leq k \leq n_Z$ . (3.22) follows from (3.21) and the fact that  $\sum_{k=1}^{n_Z} (\hat{f}_Z(z_k) - f_Z(z_k))^2$  is  $O_P(n_Z (nh_n^d)^{-1})$ . The proof of Theorem 3.1 is complete.  $\square$

**7.3. Proof of Theorem 3.2.** From Lemma 1, the joint distribution of  $\hat{V}^*(z_k) : 1 \leq k \leq n_Z$  is the same as that of  $V^*(z_k) + (nh_n^d c_K f_Z(z_k))^{-1/2} (W_{n,1,k} + W_{n,2,k}) : 1 \leq k \leq n_Z$ , where

$$(7.11) \quad \sum_{k=1}^{n_Z} \|W_{n,2,k}\|^2 = O_P(\exp(-(\ln n)^{1/9}))$$



and  $W_{n,1,k}$ 's are independent symmetric normal matrices of mean zero. To describe the covariance structure of each  $W_{n,1,k}$ , let  $\phi^* = (\phi_1^*, \dots, \phi_{p_n}^*)^T$ ,  $\psi^* = (\psi_1^*, \dots, \psi_{q_n}^*)^T$  and let  $V_0$  be the  $(p_n + q_n) \times (p_n + q_n)$  symmetric matrix such that  $g_{1,1}(V_0) = \phi^*(X)\phi^*(X)^T$ ,  $g_{1,2}(V_0) = \phi^*(X)\psi^*(Y)^T$  and  $g_{2,2}(V_0) = \psi^*(Y)\psi^*(Y)^T$ . For  $1 \leq k \leq n_Z$  and  $1 \leq m, \ell \leq p_n + q_n$ , let  $U_{k,m,\ell}$  and  $V_{0,m,\ell}$  be the  $(m, \ell)$ th elements of  $W_{n,1,k}$  and  $V_0$ , respectively, then

$$\text{Cov}(U_{k,m,\ell}, U_{k,m',\ell'}) = \text{Cov}(V_{0,m,\ell}, V_{0,m',\ell'} | Z = z_k)$$

for  $(m, \ell), (m', \ell') \in \{(i, j) : 1 \leq i \leq j \leq (p_n + q_n)\}$ . For  $1 \leq k \leq n_Z$ , let  $\tilde{V}_k = V^*(z_k) + (nh_n^d c_K f_Z(z_k))^{-1/2} (W_{n,1,k} + W_{n,2,k})$  and

$$\begin{aligned} A_1(z_k) &= g(\tilde{V}_k, \alpha^*) g_{1,1}(\tilde{V}_k) \\ &= g_{1,2}(\tilde{V}_k) (g_{2,2}(\tilde{V}_k))^{-1} g_{2,1}(\tilde{V}_k) \\ &\quad - g_{1,1}(\tilde{V}_k) \alpha^* (\alpha^*)^T g_{1,1}(\tilde{V}_k), \end{aligned}$$

and let  $\tilde{\rho}_0^2(z_k)$  be the largest eigenvalue of  $A_1(z_k)(g_{1,1}(\tilde{V}_k))^{-1}$ , then the joint distribution of  $\hat{\rho}^2(z_k) : 1 \leq k \leq n_Z$  is the same as that of  $\tilde{\rho}_0^2(z_k) : 1 \leq k \leq n_Z$ . For  $1 \leq i, j \leq 2$  and  $1 \leq k \leq n_Z$ , let  $\Delta_{i,j,k} = g_{i,j}(\tilde{V}_k) - g_{i,j}(V^*(z_k))$ , then from (7.7),

$$(7.12) \quad \sum_{k=1}^{n_Z} \sum_{i=1}^2 \sum_{j=1}^2 \|\Delta_{i,j,k}\|^2 = O_P((nh_n^d)^{-1} (\ln n)^{1/8})$$

and

$$\begin{aligned} A_1(z_k) &= g_{1,2}(V^*(z_k)) (g_{2,2}(\tilde{V}_k))^{-1} g_{2,1}(V^*(z_k)) \\ &\quad - g_{1,1}(\tilde{V}_k) \alpha^* (\alpha^*)^T g_{1,1}(\tilde{V}_k) + g_{1,2}(V^*(z_k)) \Delta_{2,1,k} \\ (7.13) \quad &+ \Delta_{1,2,k} g_{2,1}(V^*(z_k)) + \Delta_{1,2,k} \Delta_{2,1,k} \\ &\quad - g_{1,2}(V^*(z_k)) \Delta_{2,2,k} \Delta_{2,1,k} \\ &\quad - \Delta_{1,2,k} \Delta_{2,2,k} g_{2,1}(V^*(z_k)) + R_{1,n,k}, \end{aligned}$$

where

$$\begin{aligned} R_{1,n,k} &= \Delta_{1,2,k} (g_{2,2}(\tilde{V}_k)^{-1} - I_{q_n}) \Delta_{2,1,k} \\ &\quad + g_{1,2}(V^*(z_k)) (g_{2,2}(\tilde{V}_k)^{-1} - I_{q_n} + \Delta_{2,2,k}) \Delta_{2,1,k} \\ &\quad + \Delta_{1,2,k} (g_{2,2}(\tilde{V}_k)^{-1} - I_{q_n} + \Delta_{2,2,k}) g_{2,1}(V^*(z_k)). \end{aligned}$$

To simplify the expression for  $A_1(z_k)$  in (7.13), we will make use of the following properties.

(C4) The elements of the matrix  $g_{1,2}(V^*(z_k))$  are zeros except that the  $(1, 1)$ th element is 1.

- (C5) For  $(i, j) \in \{(1, 2), (2, 1)\}$ ,  $g_{i,j}(V^*(z_k))$ 's first row (or first column) is either the first row or the first column of  $g_{i',j'}(V^*(z_k))$  for  $(i', j') \neq (i, j)$ .
- (C6) The  $(1, 1)$ th element in  $g_{2,2}(\hat{V}^*(z_k))$  is 1.

Here (C4) follows from the conditional independence assumption and (3.16), and (C5) and (C6) follow from (3.15). From (C6),  $g_{2,2}(\tilde{V}_k)$  can be expressed as

$$g_{2,2}(\tilde{V}_k) = \begin{pmatrix} 1 & B_k^T \\ B_k & D_k \end{pmatrix}$$

for some matrices  $B_k$  and  $D_k$ , so the  $(1, 1)$ th element of  $g_{2,2}(\tilde{V}_k)^{-1}$  is  $(1 + B_k^T(D_k - B_k B_k^T)^{-1} B_k)^{-1}$ . Let  $J = \alpha^*(\alpha^*)^T$ , then by (C4) and (C5), we have

$$\begin{aligned} g_{1,2}(V^*(z_k))(g_{2,2}(\tilde{V}_k))^{-1} g_{2,1}(V^*(z_k)) &= (1 + B_k^T(D_k - B_k B_k^T)^{-1} B_k) J, \\ g_{1,2}(V^*(z_k)) \Delta_{2,1,k} &= J \Delta_{1,1,k} \text{ and } B_k^T B_k J = g_{1,2}(V^*(z_k)) (\Delta_{2,2,k})^2 g_{2,1}(V^*(z_k)), \end{aligned}$$

so the expression for  $A_1(z_k)$  in (7.13) becomes

$$\begin{aligned} & B_k^T ((D_k - B_k B_k^T)^{-1} - I_{q_n-1}) B_k J + g_{1,2}(V^*(z_k)) (\Delta_{2,2,k})^2 g_{2,1}(V^*(z_k)) \\ & - \Delta_{1,1,k} g_{1,2}(V^*(z_k)) g_{2,1}(V^*(z_k)) \Delta_{1,1,k} + \Delta_{1,2,k} \Delta_{2,1,k} \\ & - g_{1,2}(V^*(z_k)) \Delta_{2,2,k} \Delta_{2,1,k} - \Delta_{1,2,k} \Delta_{2,2,k} g_{2,1}(V^*(z_k)) + R_{1,n,k}. \end{aligned}$$

Let

$$\begin{aligned} A_2(z_k) &= g_{1,2}(V^*(z_k)) (g_{2,2}(W_{1,n,k}))^2 g_{2,1}(V^*(z_k)) \\ & - g_{1,1}(W_{1,n,k}) g_{1,2}(V^*(z_k)) g_{2,1}(V^*(z_k)) g_{1,1}(W_{1,n,k}) \\ & + g_{1,2}(W_{1,n,k}) g_{2,1}(W_{1,n,k}) - g_{1,2}(V^*(z_k)) g_{2,2}(W_{1,n,k}) g_{2,1}(W_{1,n,k}) \\ & - g_{1,2}(W_{1,n,k}) g_{2,2}(W_{1,n,k}) g_{2,1}(V^*(z_k)) \end{aligned}$$

and

$$\begin{aligned} R_{2,n,k} &= B_k^T ((D_k - B_k B_k^T)^{-1} - I_{q_n-1}) B_k J \\ & - (nh_n^d c_K f_Z(z_k))^{-1} A_2(z_k) + g_{1,2}(V^*(z_k)) (\Delta_{2,2,k})^2 g_{2,1}(V^*(z_k)) \\ & - \Delta_{1,1,k} g_{1,2}(V^*(z_k)) g_{2,1}(V^*(z_k)) \Delta_{1,1,k} + \Delta_{1,2,k} \Delta_{2,1,k} \\ & - g_{1,2}(V^*(z_k)) \Delta_{2,2,k} \Delta_{2,1,k} - \Delta_{1,2,k} \Delta_{2,2,k} g_{2,1}(V^*(z_k)), \end{aligned}$$

then

$$(7.14) \quad A_1(z_k) = \frac{A_2(z_k)}{nh_n^d c_K f_Z(z_k)} + R_{1,n,k} + R_{2,n,k},$$

where

$$(7.15) \quad \sum_{k=1}^{n_Z} (\|R_{1,n,k}\|^2 + \|R_{2,n,k}\|^2) = O_P \left( \frac{\exp(-(\ln n)^{1/9}) (\ln n)^{1/8}}{(nh_n^d)^2} \right)$$

from Fact 4, (7.11) and (7.12), and a simple expression for  $A_2(z_k)$  can be obtained as stated below in (C7), which follows from (C4) and (C5).

(C7) For  $1 \leq k \leq n_Z$ ,  $A_2(z_k) = C_k C_k^T$ , where  $C_k$  is the  $p_n \times q_n$  matrix obtained by replacing elements in the first row and first column of  $g_{1,2}(W_{1,n,k})$  with zeros.

Note that from (C7), we have that

$$\sum_{k=1}^{n_Z} \|A_2(z_k)\|^2 = O_P(n_Z(p_n - 1)^2(q_n - 1)^2) = O_P((\ln n)^{1/8}),$$

which, together with (7.14) and (7.15), implies that

$$(7.16) \quad \sum_{k=1}^{n_Z} \|A_1(z_k)\|^2 = O_P((nh_n^d)^{-2}(\ln n)^{1/8}),$$

and then it follows from (7.16), Fact 4 and (7.12) that

$$(7.17) \quad \sum_{k=1}^{n_Z} \|A_1(z_k)(g_{1,1}(\tilde{V}_k))^{-1} - A_1(z_k)\|^2 = O_P((nh_n^d)^{-3}(\ln n)^{1/4}).$$

For  $1 \leq k \leq n_Z$ , let  $\lambda_{0,k}$  be the largest eigenvalue of  $A_2(z_k)$  and recall that  $\tilde{\rho}_0^2(z_k)$  is the largest eigenvalue of  $A_1(z_k)(g_{1,1}(\tilde{V}_k))^{-1}$ . Then by (7.14), (7.15) and (7.17),

$$(7.18) \quad \sum_{k=1}^{n_Z} (nh_n^d c_K f_Z(z_k) \tilde{\rho}_0^2(z_k) - \lambda_{0,k})^2 = O_P(\exp(-(\ln n)^{1/9})(\ln n)^{1/8}).$$

Let  $\tilde{f}_k$ ,  $\tilde{\rho}(z_k)$  and  $\lambda_k : 1 \leq k \leq n_Z$  be random variables such that the joint distribution of  $(\tilde{f}_k, \tilde{\rho}(z_k)) : 1 \leq k \leq n_Z$  is the same as that of  $(\hat{f}_Z(z_k), \hat{\rho}(z_k)) : 1 \leq k \leq n_Z$ , and the joint distribution of  $(\tilde{\rho}(z_k), \lambda_k) : 1 \leq k \leq n_Z$  is the same as that of  $(\tilde{\rho}_0(z_k), \lambda_{0,k}) : 1 \leq k \leq n_Z$ . Note that from (7.18) and the fact that

$$\sum_{k=1}^{n_Z} \|A_2(z_k)\|^2 = O_P(n_Z(p_n - 1)^2(q_n - 1)^2),$$

we have that

$$\sum_{k=1}^{n_Z} nh_n^d c_K f_Z(z_k) \tilde{\rho}^2(z_k) = \sqrt{O_P(n_Z^2(p_n - 1)^2(q_n - 1)^2)} = O_P((\ln n)^{1/16}),$$

so  $nh_n^d \sum_{k=1}^{n_Z} (\hat{\rho}(z_k))^2 = O_P((\ln n)^{1/16})$ ,

$$\left| nh_n^d c_K \sum_{k=1}^{n_Z} \hat{f}_Z(z_k) (\hat{\rho}(z_k))^2 - nh_n^d c_K \sum_{k=1}^{n_Z} f_Z(z_k) (\hat{\rho}(z_k))^2 \right|$$

$$\begin{aligned}
&\leq nh_n^d c_K \left( \sum_{k=1}^{n_Z} (\hat{f}_Z(z_k) - f_Z(z_k))^2 \right)^{1/2} \sum_{k=1}^{n_Z} (\hat{\rho}(z_k))^2 \\
&= O_P((\ln n)^{1/16}) (O_P(n_Z (nh_n^d)^{-1}))^{1/2} \\
&= O_P((nh_n^d)^{-1/2} (\ln n)^{3/32})
\end{aligned}$$

and

$$\begin{aligned}
&\left| nh_n^d c_K \sum_{k=1}^{n_Z} \tilde{f}_k(\tilde{\rho}(z_k))^2 - \sum_{k=1}^{n_Z} \lambda_k \right| \\
&\leq O_P((nh_n^d)^{-1/2} (\ln n)^{3/32}) + \left| nh_n^d c_K \sum_{k=1}^{n_Z} f_Z(z_k)(\tilde{\rho}(z_k))^2 - \sum_{k=1}^{n_Z} \lambda_k \right| \\
&[\text{by (7.18)}] \leq O_P((nh_n^d)^{-1/2} (\ln n)^{3/32}) + \sqrt{n_Z} (O_P(\exp(-(\ln n)^{1/9}) (\ln n)^{1/8}))^{1/2} \\
&= O_P(\exp(-0.5(\ln n)^{1/9}) (\ln n)^{3/32}).
\end{aligned}$$

The proof of Theorem 3.2 is complete.

7.4. *Proof of Corollary 1.* To prove Corollary 1, it is sufficient to establish (3.25) and (3.26). To see this, let  $\tilde{f}_k$ ,  $\tilde{\rho}^2(z_k)$  and  $\lambda_k : 1 \leq k \leq n_Z$  be as in Theorem 3.2, then

$$\frac{nh_n^d c_K \sum_{k=1}^{n_Z} \hat{f}_Z(z_k) \hat{\rho}^2(z_k) - n_Z \mu_{p_n, q_n}}{\sqrt{n_Z \sigma_{p_n, q_n}^2}}$$

has the same distribution as

$$\begin{aligned}
&\frac{nh_n^d c_K \sum_{k=1}^{n_Z} \tilde{f}_k \tilde{\rho}^2(z_k) - n_Z \mu_{p_n, q_n}}{\sqrt{n_Z \sigma_{p_n, q_n}^2}} \\
&= \underbrace{\frac{nh_n^d c_K \sum_{k=1}^{n_Z} \tilde{f}_k \tilde{\rho}^2(z_k) - \sum_{k=1}^{n_Z} \lambda_k}{\sqrt{n_Z \sigma_{p_n, q_n}^2}}}_I + \underbrace{\frac{\sum_{k=1}^{n_Z} \lambda_k - n_Z \mu_{p_n, q_n}}{\sqrt{n_Z \sigma_{p_n, q_n}^2}}}_{II}.
\end{aligned}$$

Suppose that (3.25) holds, then  $I \rightarrow 0$  almost surely by (3.24) and Theorem 3.2. Also, (3.26) says that  $II$  converges to  $N(0, 1)$  in distribution. Therefore, (3.27) holds if (3.25) and (3.26) hold.

To establish (3.26), we will verify the Lyapounov condition

$$(7.19) \quad \lim_{n \rightarrow \infty} \sum_{k=1}^{n_Z} \frac{E|\lambda_k - \mu_{p_n, q_n}|^3}{(n_Z \sigma_{p_n, q_n}^2)^{3/2}} = 0,$$

and then apply Lindeberg's central limit theorem. Let  $\lambda$  be the largest eigenvalue of  $CC^T$ . Then  $\lambda \leq \text{tr}(CC^T)$ , where  $\text{tr}(CC^T)$  is the trace of  $CC^T$ , which follows the  $\chi^2$  distribution with degrees of freedom  $m_{1,n} = (p_n - 1)(q_n - 1)$ . Therefore,

$$E\lambda^3 \leq E(\text{tr}(CC^T))^3 = m_{1,n}(m_{1,n} + 2)(m_{1,n} + 4),$$

which implies that  $E|\lambda_1 - \mu_{p_n, q_n}|^3 = O(p_n^3 q_n^3)$ , so (7.19) follows from (3.25) and (3.26) holds.

It remains to prove (3.25). Consider first the case where (i) holds. By Theorem 1.1 in Johnstone [7],

$$(7.20) \quad \frac{\lambda_1 - \mu_n}{\sigma_n} \text{ converges in distribution as } n \rightarrow \infty,$$

where

$$\mu_n = (\sqrt{q_n - 2} + \sqrt{p_n - 1})^2$$

and

$$\sigma_n = (\sqrt{q_n - 2} + \sqrt{p_n - 1}) \left( \frac{1}{q_n - 2} + \frac{1}{p_n - 1} \right)^{1/3}.$$

Here the limiting distribution is the Tracy–Widom law of order 1. Let  $F$  denote its cumulative distribution function. Suppose that  $\epsilon, t_1$  and  $t_2$  are real numbers such that  $t_1 < t_1 + \epsilon < t_2 - \epsilon$ , which implies that  $F(t_2) > F(t_2 - \epsilon)$  and  $F(t_1 + \epsilon) > F(t_1)$ . From (7.20),

$$P(\lambda_1 > \mu_n + (t_2 - \epsilon)\sigma_n) \geq 1 - F(t_2)$$

and

$$P(\lambda_1 < \mu_n + (t_1 + \epsilon)\sigma_n) \geq F(t_1),$$

if  $n$  is large enough. For such  $n$ , we have

$$\sigma_{p_n, q_n}^2 \geq \frac{\min(F(t_1), 1 - F(t_2))(t_2 - t_1 - 2\epsilon)^2 \sigma_n^2}{4},$$

which gives (3.25). The proof of (3.25) for the case where (ii) holds can be done by reversing the roles of  $p_n$  and  $q_n$ . The proof of Corollary 1 is complete.

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